

CRYSTALS OF THE ALPHA 1 BETA 1 INTEGRIN I-DOMAIN
AND THEIR USE

RELATED APPLICATIONS

5 This is a continuation of PCT/US99/23261, filed on October 6, 1999 as a continuation of prior U.S. provisional Serial number 60/103,301, filed October 6, 1998. The entire disclosure of each of the aforesaid patent applications are incorporated herein by reference.

BACKGROUND OF THE INVENTION

10 A major class of cell receptors that interacts with the constituents of the extracellular matrix ("ECM") (e.g, collagen, laminin) are the integrins which are transmembrane heterodimeric glycoproteins composed of noncovalently associated α and β subunits. The integrin family contains at least 16 α subunits, seven of which contain an approximately 200 amino acid inserted domain in their N-terminal region variously called
 15 the "I-domain" or the "A-domain".

 Processes such as cell differentiation, cell proliferation and cell migration in embryonic development, as well as remodeling and cell/tissue repair events, are dependent on communication of cells with the ECM. Alpha 1 beta 1 integrin (" $\alpha 1 \beta 1$ integrin") is a cell-surface receptor for collagen I, collagen IV and laminin. It is also known as VLA-1.
 20 Indeed, $\alpha 1 \beta 1$ supports not only collagen-dependent adhesion and migration, but also is likely to be a critical collagen receptor on mesenchymally-derived cells that may be involved in ECM remodeling after injury (Gotwals et al.(1996), J. Clin. Invest. 97 : p 2469-2477). The ability of cells to contract and organize collagen matrices is a critical component of any wound healing response. Improper regulation of $\alpha 1 \beta 1$ integrin may
 25 result in certain pathological conditions such as fibrosis.

 Moreover, there is a limited, but provocative, literature suggesting that $\alpha 1 \beta 1$ may play a role in T cell/monocyte driven diseases. Anti- $\alpha 1 \beta 1$ antibodies block T-cell dependent cytokine expression. Miyake et al., J. Exp. Med., 177: 863-868 (1993). Expression of $\alpha 1 \beta 1$ is upregulated in persistently activated, 2-4 week old cultured T cells
 30 (Hemler et al., Eur. J. Immunol., 15: 502-508 (1985)) and is also expressed on a high percentage of T cells isolated from the synovium of patients with rheumatoid arthritis. Hemler et al., J. Clin. Invest., 78: 696-702 (1986). Chronic tissue damage results from both

T05940 : 91298800

resident activated T cells, and also monocytes/fibroblasts recruited by T cell-derived cytokines. Blocking the $\alpha 1\beta 1$ -induced T cell interaction might relieve tissue damage by removing activated T cells and/or by diminishing inflammatory cytokine levels.

It would therefore be useful to design, identify or obtain potential drug candidates which would interfere with the $\alpha 1\beta 1$ integrin-ECM or T-cell interaction(s). The recent emergence of drug design to identify candidates that play a role in a physiologically relevant biological pathway has provided a useful approach for obtaining, or designing, lead compounds for drugs.

Generally, this approach requires selecting a protein target molecule which plays a role in a physiologically relevant biological pathway. Typically, once an inhibitor or agonist, natural or synthesized, is found for the target molecule, it is modified or optimized to produce a candidate with the desired properties.

In order to more efficiently design or modify a ligand, it is useful to have a three-dimensional structure for the bioactive conformation of a known ligand as it binds to the target protein molecule. Furthermore, it is valuable to understand the detailed interactions of the ligand with its target protein by examining the three-dimensional structure of the protein target in complex with its known ligand. This allows the artisan to preserve the critical interactions with the protein, while modifying candidate ligands to interact more precisely with the protein, resulting in better potency and specificity.

However, the three dimensional crystal structure of the protein target is frequently unavailable due to the significant effort required to obtain crystals of sufficient size and quality to provide accurate information regarding the structure. For example, it is time consuming and often difficult to express, purify and characterize a protein. Additionally, once the protein of sufficient purity is obtained, it must be crystallized to a size and quality which is useful for x-ray diffraction and subsequent structure solution. Thus, although crystal structures can provide a wealth of valuable information in the field of drug design and discovery, crystals of certain biologically relevant molecules such as $\alpha 1\beta 1$ integrin, are not readily available to those skilled in the art.

Furthermore, although the amino acid sequence of a target protein, such as $\alpha 1\beta 1$ integrin, is known, this sequence information does not allow an accurate prediction of the crystal structure of the protein. Nor does the sequence information afford an understanding

of the structural, conformational and chemical interactions between a ligand such as $\alpha 1\beta 1$ integrin and its target.

Thus, there is a need for a detailed knowledge of the crystalline three-dimensional structure of the extracellular domain of $\alpha 1\beta 1$ integrin, to effectively design, screen or
5 optimize compounds capable of interfering with the $\alpha 1\beta 1$ integrin-ECM and/or T-cell interactions.

A soluble version of $\alpha 1\beta 1$ integrin can be made from its extracellular region or fragments thereof. As used herein, the term " $\alpha 1\beta 1$ integrin" includes soluble $\alpha 1\beta 1$ integrin polypeptides lacking transmembrane and intracellular regions, homologs and
10 analogs of $\alpha 1\beta 1$ integrin or derivatives thereof. Crystals of the $\alpha 1$ chain of $\alpha 1\beta 1$ integrin or fragments thereof of a size and quality such as described herein, would allow performance of x-ray diffraction studies and enable those skilled in the art to conduct studies relating to the binding properties of $\alpha 1\beta 1$ integrin, as well as the binding properties of molecules or molecular complexes which may associate with $\alpha 1\beta 1$ integrin or fragments thereof.

15 SUMMARY OF THE INVENTION

Accordingly, the present invention is directed to crystals of the $\alpha 1$ chain of $\alpha 1\beta 1$ integrin or crystals of fragments of the $\alpha 1$ chain, of sufficient size and quality to obtain useful information about the properties of $\alpha 1\beta 1$ integrin and molecules or complexes which may associate with it. The claimed invention provides the three-dimensional crystal
20 structure of the Cys143 to Ala340 fragment of the $\alpha 1$ chain of $\alpha 1\beta 1$ integrin, which can be used to identify binding sites to solve the structure of unknown crystals, to provide mutants having desirable binding properties, and ultimately, to design, characterize, or identify molecules or chemical entities capable of interfering with the interaction between collagen or other ligands and $\alpha 1\beta 1$.

25 Additional features and advantages of the invention will be set forth in the description which follows, and in part will be apparent from the description, or may be learned by practice of the invention. The objectives and other advantages of the invention will be realized and attained by the compositions and methods particularly pointed out in the written description and claims hereof, as well as in the appended drawings.

30 To achieve these and other advantages, and in accordance with the purpose of the invention, as embodied and broadly described herein, the invention relates to a crystal of $\alpha 1\beta 1$ integrin. More particularly, the invention relates to a crystal formed by a functional

fragment of the extracellular domain of the $\alpha 1\beta 1$ chain of $\alpha 1\beta 1$ (Cys143-Ala340), wherein the crystal has cell constants $a = 34.77\text{\AA}$, $b = 85.92\text{\AA}$, $c = 132.56\text{\AA}$, $\alpha = \beta = \gamma = 90\text{\AA}$, and a space group of $P2_12_12_1$, and equivalents of that crystal. The claimed crystals of $\alpha 1\beta 1$ are substantially described by the structural coordinates identified in Table II. The claimed

5 crystals in certain embodiments are characterized by a binding site moiety comprising Asp154, Ser156, Asn157, Ser158, Leu222, Gln223, Thr224, Asp257, Glu259, His261, His288, Tyr289, Gly292, Leu294 and Lys298. Mutants, homologs, co-complexes and fragments of the claimed crystals are also contemplated herein.

The claimed invention in certain embodiments relates to heavy atom derivatives of

10 the crystallized form of $\alpha 1\beta 1$ integrin (143-340), and, more specifically, the heavy atom derivatives of the crystallized form of $\alpha 1\beta 1$ described above. In various embodiments, the claimed invention relates to methods of preparing crystalline forms of $\alpha 1\beta 1$, or fragments thereof, by providing an aqueous solution comprising at least a fragment of $\alpha 1\beta 1$, providing a reservoir solution comprising a precipitating agent, mixing a volume of the

15 $\alpha 1\beta 1$ solution with a volume of the reservoir solution and crystallizing the resultant mixed volume. In certain embodiments, the crystal is derived from an aqueous solution comprising the $\alpha 1$ chain of $\alpha 1\beta 1$ (Cys143-Ala340). In various embodiments, the concentration of $\alpha 1\beta 1$ in the aqueous solution is about 1 to about 50 mg/ml, preferably about 5 mg/ml to about 15 mg/ml, and most preferably, about 10 mg/ml. The precipitating

20 agents used in the invention may be any precipitating agent known in the art, preferably one selected from the group consisting of sodium citrate, ammonium sulfate and polyethylene glycol. Any concentration of precipitating agent may be used in the reservoir solution, however it is preferred that the concentration be about 20% weight per volume ("w/v") to about 50% w/v, more preferably about 25% w/v. Similarly, the pH of the

25 reservoir solution may be varied, preferably between about 4 to about 10, most preferably about 6.5.

Various methods of crystallization can be used in the claimed invention, including, but not limited to, vapor diffusion, batch, liquid bridge, or dialysis. Vapor diffusion crystallization is preferred.

30 Additionally, the claimed invention relates to methods of using the claimed crystal, and the structural coordinates, in methods for screening, designing, or optimizing molecules or other chemical entities that may interfere with the interaction between $\alpha 1\beta 1$

ligands such as members of the extracellular matrix (e.g., collagen) and $\alpha 1\beta 1$. Thus, the structural coordinates of $\alpha 1\beta 1$ or portions thereof can be used to solve the crystal structure of a mutant, homologue or co-complex of $\alpha 1\beta 1$ or a fragment thereof, as well as to solve other unknown crystals which associate with $\alpha 1\beta 1$ or fragments thereof.

5 In some embodiments, the structural coordinates of the $\alpha 1$ chain of $\alpha 1\beta 1$ (as exemplified in Table II) can be used to evaluate a chemical entity to obtain information about the binding of the chemical entity to $\alpha 1\beta 1$. The structural coordinates can be used to characterize chemical entities which interfere with the relationship between the extracellular matrix (i.e., collagen or laminin) and $\alpha 1\beta 1$ such as inhibitors or agonists. The
10 coordinates can also be used to optimize binding characteristics, to determine the orientation of ligands in a binding site of $\alpha 1\beta 1$. One skilled in the art will appreciate the numerous uses of the claimed invention in the areas of drug design, screening and optimization of drug candidates, as well as in determining additional unknown crystal structures.

15 In various embodiments, the claimed invention relates to a machine readable data storage medium having a data storage material encoded with machine readable data, which, when read by an appropriate machine, can display a three dimensional representation of a crystal. The crystals displayed comprise a fragment of $\alpha 1\beta 1$ such as that described by the coordinates in Table II, or a crystal having a binding site moiety
20 comprising amino acids Asp154, Ser156, Asn157, Leu222, Gln223, Thr224, Asp257, Glu259, His261, His288, Tyr289, Gly292, Leu294 and Lys298.

In other embodiments, the claimed invention relates to a method for determining a at least a portion of a three dimensional structure of a chemical entity or molecular complex by calculating phases from the structural coordinates of a crystal of a fragment of
25 $\alpha 1\beta 1$, calculating the electron density map from the phases obtained, and then determining at least a portion of the unknown structure based upon the electron density map.

In yet other embodiments, the invention relates to methods for evaluating the ability of a chemical entity to associate with $\alpha 1\beta 1$. The methods employ computational or experimental means to perform a fitting operation between the chemical entity and the
30 $\alpha 1\beta 1$ to obtain data related to the association, and analyzing the data to determine the characteristics. Chemical entities identified by these methods which are capable of interfering with the in vivo or in vitro association between the extracellular matrix and

$\alpha 1\beta 1$ are also encompassed by the claimed invention. The claimed chemical entities may comprise binding sites substantially similar to those of $\alpha 1\beta 1$, or, alternatively may comprise binding sites capable of associating with the binding sites of $\alpha 1\beta 1$.

It is to be understood that both the foregoing general description and the following
5 detailed description are exemplary and explanatory and are intended to provide further explanation of the invention as claimed.

The accompanying drawings are included to provide a further understanding of the invention and are incorporated in and constitute a part of this specification, illustrate several embodiments of the invention, and together with the description, serve to explain
10 the principles of the invention.

BRIEF DESCRIPTION OF THE FIGURES

Figure 1: 2Fo-Fc electron density map for a representative region of the $\alpha 1$ I-domain crystal structure, contoured at 1Sigma.

Figure 2: Ribbon representation of the fold of the $\alpha 1$ I-domain molecule. The arrow points
15 to the MIDAS binding site.

DETAILED DESCRIPTION OF THE INVENTION

In order that the invention described herein may be more fully understood, the following detailed description is set forth.

The present invention relates to a crystal of a soluble fragment of the extracellular
20 domain of the $\alpha 1\beta 1$ integrin. Specifically, it relates to a crystal of a soluble protein comprising the sequence from Cys143 to Ala340 of the $\alpha 1$ chain of $\alpha 1\beta 1$ integrin (" $\alpha 1\beta 1(143-340)$ "), the structure of $\alpha 1\beta 1(143-340)$ as determined by X-ray crystallography, and the use of the $\alpha 1\beta 1(143-340)$ structure and that of its homologs, mutants and co-complexes to design, identify, characterize, screen and/or optimize
25 candidate inhibitors or agonists of $\alpha 1\beta 1$ activity.

A. DEFINITIONS

The term $\alpha 1\beta 1$ integrin ("VLA-1" or " $\alpha 1\beta 1$ " or " $\alpha 1\beta 1$ integrin", used interchangeably) herein refers to a genus of polypeptides which are capable of binding to members of the extracellular matrix proteins such as laminin or collagen, or homologs or
30 fragments thereof. The term as used herein includes $\alpha 1\beta 1$ integrin 143-340), homologs, mutants, equivalents and fragments thereof.

The term "co-complex" refers to an $\alpha 1\beta 1$ or a mutant or homolog of $\alpha 1\beta 1$ in covalent or non-covalent association with a chemical entity.

The term "homolog" or "homologous"- as used herein is synonymous with the term "identity" and refers to the sequence similarity between two polypeptides, molecules or
5 between two nucleic acids. When a position in both of the two compared sequences is occupied by the same base or amino acid monomer subunit (for instance, if a position in each of the two DNA molecules is occupied by adenine, or a position in each of two polypeptides is occupied by a lysine), then the respective molecules are homologous at that position. The percentage homology between two sequences is a function of the number of
10 matching or homologous positions shared by the two sequences divided by the number of positions compared x 100. For instance, if 6 of 10 of the positions in two sequences are matched or are homologous, then the two sequences are 60% homologous. By way of example, the DNA sequences CTGACT and CAGGTT share 50% homology (3 of the 6 total positions are matched). Generally, a comparison is made when two sequences are
15 aligned to give maximum homology. Such alignment can be provided using, for instance, the method of Needleman et al., *J. Mol Biol.* 48: 443-453 (1970), implemented conveniently by computer programs such as the Align program (DNASTar, Inc.). Homologous sequences share identical or similar amino acid residues, where similar residues are conservative substitutions for, or "allowed point mutations" of, corresponding
20 amino acid residues in an aligned reference sequence. In this regard, a "conservative substitution" of a residue in a reference sequence are those substitutions that are physically or functionally similar to the corresponding reference residues, e.g., that have a similar size, shape, electric charge, chemical properties, including the ability to form covalent or hydrogen bonds, or the like. Particularly preferred conservative substitutions are those
25 fulfilling the criteria defined for an "accepted point mutation" in Dayhoff et al., 5: **Atlas of Protein Sequence and Structure**, 5: Suppl. 3, chapter 22: 354-352, Nat. Biomed. Res. Foundation, Washington, D.C. (1978).

The term "mutant" refers to an $\alpha 1\beta 1$ integrin or fragment thereof, characterized by the replacement, deletion, or insertion of at least one amino acid from the wild-type. Such
30 a mutant may be prepared, for example, by expression of $\alpha 1\beta 1$ integrin previously altered in its coding sequence by oligonucleotide-directed mutagenesis.

The term “positively charged amino acid” includes any amino acid, natural or unnatural, having a positively charged side chain under normal physiological conditions. Examples of positively charged naturally occurring amino acids are arginine, lysine and histidine.

- 5 The term “negatively charged amino acid” includes any amino acid, natural or unnatural, having a negatively charged side chain under normal physiological conditions. Examples of negatively charged naturally occurring amino acids are aspartic acid and glutamic acid.

- 10 The term “hydrophobic amino acid” means any amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples are alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophane and methionine.

 The term “hydrophilic amino acid” means any amino acid having an uncharged, polar side chain that is relatively soluble in water. Examples are serine, threonine, tyrosine, asparagine, glutamine, and cysteine.

- 15 The term “altered surface charge” means a change in one or more of the charge units of a mutant polypeptide, at physiological pH, as compared to $\alpha 1\beta 1$ integrin. The change in surface charge can be determined by measuring the isoelectric point (pI) of the polypeptide molecule containing the substituted amino acid and comparing it to the pI of the wild-type molecule.

- 20 The term “associating with” refers to a condition of proximity between two chemical entities, or portions thereof, for example, an $\alpha 1\beta 1$ integrin or portions thereof and a chemical entity. The association may be non-covalent, wherein the juxtaposition is energetically favored by hydrogen bonding, van der Waals interaction, or electrostatic interaction, or it may be a covalent association.

- 25 The term “binding site” refers to any or all of the sites where a chemical entity binds or associates with another entity.

- The term “structural coordinates” refers to the coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of molecule in crystal form. The
30 diffraction data are used to calculate an electron density map of the repeating units of the crystal. Those skilled in the art will understand that the data obtained are dependent upon the particular system used, and hence, different coordinates may in fact describe the same

crystal if such coordinates define substantially the same relationship as those described herein. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

Those of skill in the art understand that a set of structural coordinates determined by X-ray crystallography is not without standard error. Table II is the atomic coordinates of the I-domain of the $\alpha 1\beta 1$ chain of $\alpha 1\beta 1$ integrin (143-340). For the purpose of this invention, any set of structural coordinates of $\alpha 1\beta 1$ (143-340) that have a root mean square deviation of equivalent protein backbone atoms of less than about 2Å when superimposed-- using backbone atoms-- on the structural coordinates in Table II shall be considered identical. Preferably the deviation is less than about 1Å and more preferably less than about 0.5Å.

The term "heavy atom derivatization" refers to a method of producing a chemically modified form of a crystallized $\alpha 1\beta 1$ integrin. In practice, a crystal is soaked in a solution containing heavy metal atom salts, or organometallic compounds, e.g., lead chloride, gold thiomalate, thimerosal or uranyl acetate, which can diffuse through the crystal and bind to the surface of the protein. The location of the bound heavy metal atom(s) can be determined by X-ray diffraction analysis of the soaked crystal. This information can be used to generate the phase information used to construct the three-dimensional structure of the molecule.

The term "unit cell" refers to a basic shaped block. The entire volume of a crystal may be constructed by regular assembly of such blocks. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

The term "space group" refers to the arrangement of symmetry elements of a crystal.

The term "molecular replacement" refers to a method that involves generating a preliminary structural model of a crystal whose structural coordinates are unknown, by orienting and positioning a molecule whose structural coordinates are known e.g. the $\alpha 1$ I-domain coordinates in Table II, within the unit cell of the unknown crystal, so as to best account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model, and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This in turn can be subject to any of the several forms of refinement to provide a final accurate

structure of the unknown crystal. See, e.g., Lattman, E., "Use of the Rotation and Translation Functions", Methods in Enzymology, 115, pp. 55-77 (1985); Rossman, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser. No. 13, Gordon and Breach, New York (1972), all specifically incorporated by reference herein. Using the structural
5 coordinates provided by this invention, molecular replacement may be used to determine the structural coordinates of a crystalline co-complex, unknown ligand, mutant, homolog, or of a different crystalline form of $\alpha 1\beta 1$ or fragment thereof. Additionally, the claimed crystal and its coordinates may be used to determine the structural coordinates of a chemical entity which associates with $\alpha 1\beta 1$ or fragment or with a member of the
10 extracellular matrix which is a ligand for $\alpha 1\beta 1$ or fragment thereof.

The term "chemical entity" as used herein shall mean, for example, any molecule, molecular complex, compound or fragment thereof.

Mutants of $\alpha 1\beta 1$ or fragments thereof may be generated by site-specific incorporation of natural or unnatural amino acids into $\alpha 1\beta 1$ or fragments using general
15 biosynthetic methods known to those skilled in the art. For example, the codon encoding the amino acid of interest in wild-type $\alpha 1$ chain of $\alpha 1\beta 1$ may be replaced by a "blank" nonsense codon, such as TAG, using oligonucleotide-directed mutagenesis. A suppressor tRNA directed against this codon can then be chemically aminoacylated in vitro with the desired amino acid. The aminoacylated tRNA can then be added to an in vitro translation
20 system to yield a mutant $\alpha 1\beta 1$ with the site-specific incorporated amino acid.

The term "soluble fragment" of $\alpha 1\beta 1$ and any equivalent term used herein, refers to a functional fragment of $\alpha 1\beta 1$, and more particularly refers to a functional $\alpha 1$ chain. The term "functional" as used in this context refers to a soluble fragment of the extracellular domain that is capable of binding to, or associating with a member of the extracellular
25 matrix such as collagen or laminin or any fragments or homologs thereof, including molecular complexes comprising fragments thereof. Such binding may be demonstrated through immunoprecipitation experiments, using standard protocols known in the art.

A. ALPHA 1 BETA 1 INTEGRIN, its Crystal, and its Biological Implications

It will be understood that throughout the specification and claims, the positional
30 location of the amino acids described is not an absolute value, but rather, defines the relative relationship of the residues. Thus it is intended that the present invention encompass the sequences having the same or similar relative positions.

For the first time, the present invention permits the use of molecular design techniques to design, screen and optimize chemical entities and compounds, including inhibitory compounds, capable of binding to the active site or accessory binding site of $\alpha 1\beta 1$, in whole or in part. The $\alpha 1\beta 1$ integrin is a membrane-bound protein of considerable biomedical interest because of its involvement in important functions mediated by its binding to the extracellular matrix such as collagen. Since $\alpha 1\beta 1$ is found in various vertebrate (e.g., mammalian) organisms, such as humans, mice, rats, and pigs, the claimed invention is not intended to be limited to any particular species or organism.

The $\alpha 1\beta 1$ integrin (VLA-1) is a member of the integrin family of proteins. The crystal structure of I-domains from other members of this family, αM , αL and $\alpha 2$, have been described. See Dickeson & Santoro (1998) Cell. Mol. Life Sci. 54, 556-566 for a review and Emsley et al., J. Biol.Chem. 272, 28512-28517.

These I-domains were used as a framework for understanding the $\alpha 1\beta 1$ integrin(143-340) crystal structure. However, despite certain similarities, the differences between the I-domain of $\alpha 1$ and the I-domains of αM , αL , and $\alpha 2$ integrins, confirm that these ligand-receptor systems utilize spatially overlapping, but nonidentical and nonconserved sites of contact residues with different molecular determinants of binding.

Considering the complexity and overlap of the various integrins and their biological processes, the fact that $\alpha 1\beta 1$ binds specifically to its ligand suggests that inhibiting $\alpha 1\beta 1$ signaling may have important therapeutic applications. The crystal structure of $\alpha 1\beta 1$ (143-340) presented here is expected to be useful in the design, identification, characterization and optimization of such therapeutic agents.

The following detailed description of applicants invention encompasses the (a) crystal structure of the $\alpha 1$ chain I-domain (Cys143-Ala340) of $\alpha 1\beta 1$ integrin and the coordinates thereof, (b) the binding sites thereof, (c) methods of making an $\alpha 1\beta 1$ crystal or fragment thereof, and (d) methods of using the $\alpha 1\beta 1$ crystal or fragment thereof and its structural coordinates.

(a) Crystal Structure of the $\alpha 1$ I-domain

The claimed invention provides crystals of $\alpha 1\beta 1$ integrin as well as the structure derived therefrom. The crystals are derived from the $\alpha 1$ I-domain of the rat. Nevertheless, the sequence identity between rat and human alpha 1 I-domains is about 95%. Specifically, the amino acids which differ between the rat and human $\alpha 1$ I-domains are

Ile166, Asn214, Gly217, Arg 218, Gln219 Leu222, Tyr262, Gln267, His288, Ala330 (rat I-domain sequence). Most of them are located a relatively long distance away from the metal-ion-dependent-adhesion-site (MIDAS) of the $\alpha 1$ I-domain, the site likely to be involved in ligand binding. The only 2 amino acids that are expected to participate in ligand binding are the Leu222 and His288. This high degree of primary amino acid sequence identity indicates that the 3-dimensional structures of rat and human 1 I-domains are expected to be similar. Therefore, we used the crystal structure of the rat 1 I-domain for the purposes discussed in this patent and we fully expect that the 3-dimensional structure of the human 1 I-domain will have substantially identical coordinates for the main chain atoms.

The claimed invention provides crystals of a fragment from the $\alpha 1$ chain of $\alpha 1\beta 1$ integrin(143-340) having unit cells which are rhombohedral, and having the following dimensions $a = 34.77\text{\AA}$; $b = 85.92\text{\AA}$ and $c = 132.56\text{\AA}$; $\alpha = \beta = \gamma = 90\text{\AA}$. Almost all of the residues of the I-domain of the $\alpha 1$ chain of $\alpha 1\beta 1$ integrin, except for residues 143-144 of the N terminus and 336-340 of the C-terminus, are well defined in the final electron density map shown in Figure 1. The current model consists of 386 amino acid residues and 199 water molecules with a crystallographic R factor of 23.5 % and an R_{free} of 30.2% for data between 100\AA and 2.2\AA .

There are two copies of the molecule (termed "A" and "B") in the asymmetric unit. The Ramachandran diagram shows that 384 out of the 386 amino acid residues have (ϕ, ψ) angles within the allowed regions. The exception is residue Glu192 (A & B). In the atomic coordinates of the rat I-domain crystal structure (Table II), residues Thr145, Gln146, Arg234 of molecule A and Thr145 and Arg175 of molecule B are modeled as alanines because of absence of electron density for the side chain. In addition, residues 143, 145, 337, 338, 339, 340 of molecule A and 143, 144, 339, 340 of molecule B are not included in the model due to weak electron density.

The I-domain adopts the nucleotide-binding fold (Figure 2) characterized by the existence of seven helices surrounding a core of five parallel β -strands and one antiparallel β -strand. The dimensions of the molecule are $25\text{\AA} \times 30\text{\AA} \times 50\text{\AA}$. The overall fold is similar to that of αM , αL and $\alpha 2$ I-domains and in particular to that of the $\alpha 2$ I-domain. By homology to the other I-domains it is inferred that the metal-ion-dependent-adhesion-site (MIDAS) of the $\alpha 1$ I-domain consists of residues Asp154, Ser156, Ser158, Thr224, Asp

257. The MIDAS site is the site of Mg or Mn cation binding and is expected to be involved in ligand binding. The crystals were grown in the absence of Mg or Mn cations (except for contaminants) and there is no electron density visible in that would correspond to a cation. The structure appears to have the "inactive" conformation according to the model proposed in Lee et al. (1995) Structure 3, 1333-1340. The conformations of molecules A and B are very similar.

(b) Binding Sites

Modeling studies done for collagen binding on the $\alpha 2$ I-domain (Emsley et al. (1997) J. Biol.Chem. 272, 28512-28517) suggest that the binding site for collagen is expected to include the MIDAS site as well as several neighboring residues. By analogy, the binding site of the $\alpha 1$ I-domain for collagen is expected to include residues Asp154, Ser156, Asn157, Ser158, Leu222, Gln223, Thr224, Asp257, Glu259, His261, His288, Tyr289, Gly292, Leu294 and Lys298. Of interest is the observation that the MIDAS site of the $\alpha 1$ I-domain (molecule A in the crystal) forms an interaction with Arg246 of molecule B. It is possible that the positive charge of the arginine side chain replaces the positive charge of the missing metal ion.

(c) Methods of Making an $\alpha 1\beta 1$ Crystal

In various embodiments, the claimed invention relates to methods of preparing crystalline forms of $\alpha 1\beta 1$, or fragments thereof by first providing an aqueous solution comprising $\alpha 1\beta 1$ or a fragment of $\alpha 1\beta 1$. A reservoir solution comprising a precipitating agent is then mixed with a volume of the $\alpha 1\beta 1$ solution and the resultant mixed volume is then crystallized. In certain embodiments, the crystal is derived from an aqueous solution comprising $\alpha 1\beta 1$ (127-340). In preferred embodiments, the crystal is derived from an aqueous solution comprising $\alpha 1\beta 1$ (143-340). The concentration of $\alpha 1\beta 1$ or fragment in the aqueous solution may vary, and is preferably about 1 to about 50 mg/ml, more preferably about 5 mg/ml to about 15 mg/ml, and most preferably, about 10 mg/ml. Similarly, precipitating agents used in the invention may vary, and may be selected from any precipitating agent known in the art. Preferably the precipitating agent is selected from the group consisting of sodium citrate, ammonium sulfate and polyethylene glycol, with polyethylene glycol 8000 being most preferred. Any concentration of precipitating agent may be used in the reservoir solution, however it is preferred that the concentration be about 20% w/v to about 35%w/v, more preferably about 25% w/v. The pH of the

reservoir solution may also be varied, preferably between about 4 to about 10, most preferably about 6.5. One skilled in the art will understand that each of these parameters can be varied without undue experimentation and acceptable crystals will still be obtained. In practice, once the appropriate precipitating agents, buffers or other experimental
5 variables are determined for any given growth method, any of these methods or any other methods can be used to grow the claimed crystals. One skilled in the art can determine the variables depending upon his particular needs.

Various methods of crystallization can be used in the claimed invention, including, but not limited to, vapor diffusion, batch, liquid bridge, or dialysis. Vapor diffusion
10 crystallization is preferred. See, e.g. McPherson et al., "Preparation and Analysis of Protein Crystals", Glick, Ed., pp 82-159, John Wiley & Co. (1982); Jancarik et.al., "Sparse matrix sampling: a screening method for crystallization of protein", J. Appl. Cryst. 24, 409-411 (1991), specifically incorporated by reference herein.

In vapor diffusion crystallization, a small volume (i.e. a few milliliters) of protein
15 solution is mixed with a solution containing a precipitating agent. This mixed volume is suspended over a well containing a small amount, i.e. about 1 ml, of precipitating solution. Vapor diffusion from the drop to the well will result in crystal formation in the drop.

The dialysis method of crystallization utilizes a semipermeable size exclusion membrane which retains the protein but allows small molecules (i.e. buffers and
20 precipitating agents) to diffuse in and out. In dialysis, rather than concentrating the protein and the precipitating agent by evaporation, the precipitating agent is allowed to slowly diffuse through the membrane and reduce the solubility of the protein while keeping the protein concentration fixed.

The batch methods generally involve the slow addition of a precipitating agent to
25 an aqueous solution of protein until the solution just becomes turbid, at this point the container can be sealed and left undisturbed for a period of time until crystallization occurs.

Thus, applicants intend that the claimed invention encompass any and all methods of crystallization. One skilled in the art can choose any of such methods and vary the
30 parameters such that the chosen method results in the desired crystals.

(d) Use of ALPHA 1 BETA 1 INTEGRIN Crystal and its Coordinates

The claimed crystals, and coordinates describing them, permit the use of molecular design techniques to design, select and synthesize chemical entities and compounds, including inhibitory compounds or agonists capable of binding to, or associating with, the binding site of $\alpha 1\beta 1$ integrin in whole or in part.

5 One approach enabled by this invention is the use of the structural coordinates defined herein to design chemical entities that bind to or associate with, $\alpha 1\beta 1$ or fragments of $\alpha 1\beta 1$ and alter the physical properties of the compounds in different ways. Thus, properties such as, for example, solubility, affinity, specificity, potency, on/off rates or other binding characteristics may all be altered and/or optimized.

10 One may design desired chemical entities by probing a crystal of the present invention with a library of different entities to determine optimal sites for interaction between candidate chemical entities and $\alpha 1\beta 1$ or fragments of $\alpha 1\beta 1$. For example, high resolution x-ray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule sticks. Small molecules that bind
15 tightly to those sites can then be designed and synthesized and tested for the desired activity. Once the desired activity is obtained, the molecules can be further optimized.

 The claimed invention also makes it possible to computationally screen small molecule data bases or computationally design chemical entities or compounds that can bind in whole, or in part, to extracellular matrix proteins or $\alpha 1\beta 1$ or fragments thereof.
20 They may also be used to solve the crystal structure of mutants, co-complexes, or of the crystalline form of any other molecule homologous to, or capable of associating with, at least a portion of $\alpha 1\beta 1$, i.e., the I-domain of the $\alpha 1$ chain.

 One method that may be employed for this purpose is molecular replacement. An unknown crystal structure, which may be any unknown structure, such as, for example,
25 another crystal form of $\alpha 1\beta 1$, an $\alpha 1\beta 1$ mutant, or a co-complex with an extracellular matrix protein such as laminin or collagen, or any other unknown crystal of a chemical entity which associates with $\alpha 1\beta 1$ or fragment which is of interest, may be determined using the structural coordinates of this invention, set forth in Table II. Co-complexes with $\alpha 1\beta 1$ or fragments may include, but are not limited to, laminin- $\alpha 1\beta 1$, collagen- $\alpha 1\beta 1$, and
30 “small molecule”- $\alpha 1\beta 1$. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information without the claimed invention. The information obtained can thus be used to

optimize potential inhibitors or agonists of $\alpha 1\beta 1$, and more importantly, to design and synthesize novel classes of chemical entities which will affect the relationship between $\alpha 1\beta 1$ and its ligand(s) in the extracellular matrix.

The design of compounds that inhibit or agonize $\alpha 1\beta 1$ according to this invention generally involves consideration of at least two factors. First, the compound must be capable of physically or structurally associating with $\alpha 1\beta 1$ or a fragment thereof. The association may be any physical, structural, or chemical association, such as, for example, covalent or noncovalent bonding, van der Waals interactions, hydrophobic or electrostatic interactions.

Second, the compound must be able to assume a conformation that allows it to associate with $\alpha 1\beta 1$ or fragment thereof. Although not all portions of the compound will necessarily participate in the association with $\alpha 1\beta 1$ or fragment, those non-participating portions may still influence the overall conformation of the molecule. This in turn may have a significant impact on the desirability of the compound. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site.

The potential inhibitory or binding effect of a chemical compound on $\alpha 1\beta 1$ or fragment may be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and $\alpha 1\beta 1$ or its fragment(s), the need for synthesis and testing of the compound is obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to $\alpha 1\beta 1$ or fragment thereof. Thus, expensive and time consuming synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of $\alpha 1\beta 1$ or fragment may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the individual binding sites of $\alpha 1\beta 1$.

Thus, one skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with $\alpha 1\beta 1$ and more particularly, with the individual binding sites of the I-domain of the $\alpha 1$ chain of $\alpha 1\beta 1$ (143-340). This process may begin by visual inspection of, for example, the binding site on a computer screen

based on the coordinates in Table II. Selected fragments or chemical entities may then be positioned in a variety of orientations, or “docked”, within an individual binding pocket of $\alpha 1\beta 1$. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

Specialized computer programs may be of use for selecting interesting fragments or chemical entities. (GRID, available from Oxford University, Oxford, UK; MCSS or CATALYST, available from Molecular Simulations, Burlington, MA; AUTODOCK, available from Scripps Research Institute, La Jolla, CA; DOCK available from University of California, San Francisco, CA., XSITE, University College of London, UK.)

Once suitable chemical entities or fragments have been selected, they can be assembled into an inhibitor or agonist. Assembly may be by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen, in relation to the structural coordinates disclosed herein.

Alternatively, one may design the desired chemical entities “de novo”, experimentally, using either an empty binding site, or optionally including a portion of a molecule with desired activity. Thus, for example, one may use solid phase screening techniques where either $\alpha 1\beta 1$ or a fragment thereof, or candidate chemical entities to be evaluated are attached to a solid phase thereby identifying potential binders for further study or optimization.

Basically, any molecular modeling techniques may be employed in accordance with the invention; these techniques are known, or readily available to those skilled in the art. It will be understood that the methods and compositions disclosed herein can be used to identify, design or characterize not only entities which will associate or bind to $\alpha 1\beta 1$ or fragment thereof, but alternatively to identify, design or characterize entities which, like $\alpha 1\beta 1$, will bind to extracellular matrix proteins, thereby disrupting the $\alpha 1\beta 1$ -ECM interaction. The claimed invention is intended to encompass these methods and compositions broadly.

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to $\alpha 1\beta 1$ or fragment thereof may be tested and optimized using computational or experimental evaluation. Various parameters can be optimized depending on the desired result. These include, but are not limited to,

specificity, affinity, on/off rates, hydrophobicity, solubility and other characteristics readily identifiable by the skilled artisan. Thus, one may optionally make substitutions, deletions, or insertions in some of the components of the chemical entities in order to improve or modify the binding properties. Generally, initial substitutions are conservative, i.e the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original component.

The present invention also enables the design of mutants of $\alpha 1\beta 1$ and the solving of their crystal structure. More particularly, the claimed invention enables one skilled in the art to determine the location of binding sites and interfaces, particularly in the I-domain of the $\alpha 1$ chain. thereby identifying desirable sites for mutation.

For example, mutation may be directed to a particular site or combination of sites on the I-domain, by replacing or substituting one or more amino acid residues. Such mutants may have altered binding properties which may or may not be desirable.

The mutants may be prepared by any methods known in the art, such as for example, site directed mutagenesis, deletion or addition, and then tested for any properties of interest. For example, mutants may be screened for an altered charge at a particular pH, tighter binding, better specificity etc.

Additionally, the claimed invention is useful for the optimization of potential small molecule drug candidates. Thus, the claimed crystal structures can be also be used to obtain information about the crystal structures of complexes of the $\alpha 1\beta 1$ integrin and small molecule inhibitors. For example, if the small molecule inhibitor is co-crystallized with $\alpha 1\beta 1$ or a fragment thereof, then the crystal structure of the complex can be solved by molecular replacement using the known coordinates of $\alpha 1\beta 1$ or fragment for the calculation of phases. Such information is useful, for example, for determining the nature of the interaction between the I-domain of $\alpha 1\beta 1$ integrin and the small molecule inhibitor, and thus, may suggest modifications which would improve binding characteristics such as affinity, specificity and kinetics.

Example 1: Determination of Crystal Structure of the ALPHA 1 INTEGRIN I-DOMAIN (127-340)

A. Expression and purification of $\alpha 1$ integrin I-domain.

A soluble fragment of the extracellular domain of rat integrin $\alpha 1\beta 1$ $\alpha 1$ chain containing amino acid residues Val127 to the C-terminal residue Ala340 was produced in

soluble form and purified as follows: The gene encoding the rat $\alpha 1\beta 1$ I-domain sequence of amino acids Val127-Ala340 of the $\alpha 1$ chain was amplified from full length cDNAs by the polymerase chain reaction (PCR) (PCR CORE Kit; Boehringer Mannheim, GmbH Germany), using rat specific primers (5'-CAGGATCCGTCAGTCCTACATTTCAA-3'

5 [forward][SEQ ID NO: 1]; 5'-TCCTCGAGCGCTTCCAAAGCGAATAT-3'
[reverse][SEQ ID NO: 2] .

The resulting PCR amplified products were purified over a PCR select II column (5 prime-3 prime), digested with Bam H1 and Xho 1 restriction enzymes, re-purified over a PCR select II column, and ligated in pGEX4t (Pharmacia), previously digested with
10 Bam H1 and Xho1, dephosphorylated with calf intestinal alkaline phosphatase (New England Biolabs), and gel purified. Ligation products were transformed into competent DH5A E.Coli cells (Gibco BRL) and the resulting ampicillin resistant colonies were screened for the expression of the ~45 kDa glutathione S-transferase-I domain fusion protein. The I-domain was expressed as a GST fusion protein with a thrombin cleavage site
15 at the junction of the sequences.

Cells in PBS (1 part of wet cell weight to 4 parts of buffer) were lysed in a Gaulin press and clarified of particulates by centrifugation (14,000 x g, 30 min). 650 ml of lysate from 180 g of cell paste was loaded onto a 25 ml glutathione Sepharose 4B column (Pharmacia). The column was washed with 100 ml of PBS and the rat $\alpha 1$ integrin I
20 domain-GST fusion protein eluted from the column with 50 mM Tris HCl pH 8.0, 5 mM glutathione (reduced). Five ml fractions were collected and analyzed for total protein by absorbance at 280 nm and for purity by SDS-PAGE. Peak fractions were pooled, aliquoted, and stored at -70 degrees C. A total of 375 mg of the fusion protein (15 mg/ml) at >90% purity was recovered.

25 For preparation of the purified I-domain, 6 ml of the fusion protein was dialyzed overnight against one liter of 50 mM Tris pH 7.5. The sample was treated with 100 μ g of thrombin (a gift of Dr. John Fenton, New York State Department of Health, Albany, NY) for 150 min at room temperature. DTT was added to 2 mM and the sample was loaded onto a 7 ml glutathione Sepharose® 4B column. The flow through from the column was
30 collected as 1.5 ml fractions and the column was further washed with 50 mM Tris HCl pH 7.5, 2 mM DTT buffer. The flow through and wash fractions were analyzed for

absorbance at 280 nm. Peak fractions were pooled and loaded onto a 2.4 ml Q Sepharose® FF column (Pharmacia).

The Q-Sepharose column was washed with 2 ml of 50 mM Tris HCl pH 7.5, 2 mM DTT; 2 ml of 50 mM Tris HCl pH 7.5, 10 mM 2-mercaptoethanol; twice with 2ml of 50 mM Tris HCl pH 7.5, 10 mM 2-mercaptoethanol, 25 mM NaCl; and the alpha 1 integrin I domain eluted with 50 mM Tris HCl pH 7.5, 10 mM 2-mercaptoethanol, 75 mM NaCl. Peak fractions were pooled, filtered through a 0.2 µm filter, and stored at 4 degrees C. The final product was >99% pure by SDS-PAGE, eluted as a single peak by size exclusion chromatography on a Superose® 6 column (Pharmacia & Upjohn) consistent with its predicted mass, and by electrospray ionization-mass spectrometry (ESI-MS, Micromass, Quattro-II, Manchester, UK) contained a single ion with mass of 24,868 Da, which agreed with the predicted mass of 24871.2 Da for the rat α1 I-domain sequence plus the GS linker resulting from cleavage at the engineered thrombin cleavage site. From 72 mg of the fusion protein, 24 mg of the purified I- domain was recovered (based on a theoretical extinction coefficient of 0.5 at 280 nm for 1 mg/ml solution of the I-domain).

In preliminary studies, we found that the rat α1 integrin I-domain in this form failed to crystallize under any test condition and, as had been observed for other I domains (R.Liddington, personal communication), that sequences at the N-terminus of the I domain construct were problematic. A simple proteolytic method was developed to convert the purified rat I-domain into a form that could be crystallized.

Briefly, 240 µl of the purified alpha 1 integrin I domain (16 mg/ml) was diluted with 360 µl of 50 mM Tris HCl pH 7.5 and loaded onto a 1.2 ml V8 protease column (Pierce) that had been equilibrated in 50 mM Tris HCl pH 7.5. The I domain solution was left in contact with the resin for 35 min at room temperature and then recovered by washing the column with 50 mM Tris HCl pH 7.5. The I domain was then dialyzed overnight against 10 mM Tris pH 7.5, 10 mM 2-mercaptoethanol and concentrated to 11 mg/ml in a centricon-10 ultrafiltration unit (Amicon). ESI-MS analysis of V8 protease digested product revealed that the product had been converted into a des 1-18 form, starting at Cys143 in the fusion protein construct.

B. Crystallization

Buffer chemicals were purchased from Fisher (Boston, MA). Crystallization condition screenings were done with the Crystal Screen I kit from Hampton Research

(Riverside, CA). Crystals were grown by the vapor diffusion method of Jancarik & Kim (1991) J. Appl. Crystallogr. 24, 409-411.

In order to find conditions of crystallization, an incomplete factorial screen was set up. In a typical experiment, protein solution was mixed with an equal volume of reservoir solution and a drop of the mixture was suspended under a glass cover slip over the reservoir solution. Crystals were grown out of 25% w/v Polyethylene Glycol (PEG) 8000, 0.1 M sodium cacodylate pH 6.5, 0.2 M sodium acetate reservoir solution. The crystals are shaped as plates, are easy to reproduce and can reach maximum dimensions of almost 0.5 mm on one side. Variation of pH between 6 and 7 did not affect crystal quality.

Those of skill in the art will appreciate that the aforesaid crystallization conditions can be varied. By varying the crystallization conditions, other crystal forms of $\alpha 1\beta 1$ integrin I-domain may be obtained. Such variations may be used alone or in combination, and include: varying final protein concentrations between 5 mg/ml and 35 mg/ml; varying the $\alpha 1\beta 1$ integrin I-domain to precipitant ratio; varying PEG concentrations between 15% and 35% w/v; varying the molecular weight of polyethylene glycol from 400 to 8000; varying pH ranges between 5.0 and 9.5; varying sodium cacodylate concentrations between 5 and 395 mM; varying sodium acetate concentrations between 5 and 495 mM; varying the concentration or type of detergent; varying the temperature between -5 degrees C and 30 degrees C; and crystallizing $\alpha 1\beta 1$ integrin I-domain by batch, liquid bridge, or dialysis method using the above conditions or variations thereof. See McPherson, A.(1982). Preparation and Analysis of Protein Crystals. (Glick, ed.) pp. 82-159, John Wiley & Co., N.Y., specifically incorporated by reference herein.

C. Data collection and processing

Crystals were equilibrated gradually in a cryoprotectant solution of 20% glycerol, 25% w/v PEG 8000, 0.1 M sodium cacodylate pH 6.5, 0.2 M sodium acetate, and were mounted on a loop and immediately frozen in a -150 C liquid nitrogen gas stream. The technique of freezing the crystals essentially immortalizes them and produced a much higher quality data set.

A native X-ray data set up to 3.0 Å resolution was collected from one crystal by using an R-AXIS II image plate detector system (Molecular Structure Corporation, Woodlands, TX). A second data set to 2.2 Å resolution was collected later by using a

larger crystal. The data were integrated and reduced using the HKL program package (Otwinowski et al (1993) in Data collection and Processing pp 80-86, SERC Daresbury Laboratory, Warrington, UK). The data collection required about 4 days. Data processing suggested an orthorhombic unit cell with approximate cell dimensions $a=34.77$ Å, $b=85.92$ c=132.56 and $\alpha=\beta=\gamma=90$. The space group was identified as $P2_12_12_1$. The 2.2 Å data set was 91.3% complete and had an R-merge of 5.6%. Calculation of the Matthews volume gives $V_M = 4.22$ assuming a molecular weight of 23,000 daltons which suggested that there are 2 molecules in the asymmetric unit.

D. Molecular replacement

All subsequent molecular replacement computing was done with the program Amore (Navaja et al (1994) Acta Crystallogr. A 50, 157-163) from the CCP4 program package (The SERC (UK) Collaborative Computing Project No 4, Daresbury Laboratory, UK 1979). Molecular graphics manipulations were done with QUANTA (Molecular Simulations, Inc.) and "O" software (Jones et al 1991 Acta Crystallogr. A 47, 110-119). The coordinates of the crystal structure of the human $\alpha 2$ I-domain (Emsley et al. (1997) J. Biol.Chem. 272, 28512-28517) was used as a probe for rotation and translation searches using the 3 Å data set.

We used all the coordinates of all atoms, including side chains. The rotation function gave a solution with the highest correlation coefficient (cc) of 9.7. This solution was used for a first translation function which yielded a cc of 24.6 and an R-factor of 48.7%. Using rigid body refinement, these values refined to cc=40.3, R-factor=48.7%. Using this first solution, we took the peaks of the first rotation search and used these for searching the second molecule, keeping our first solution fixed. The translation search yielded a maximum peak with cc=37.3 and an R-factor of 44.8%. Rigid body refinement on these two solutions resulted in cc=56.3 and R-factor=43.3%.

The next highest solution gave: cc=36.6 R-fac=49.9%. By generating symmetry related molecules and displaying them with computer graphics it was found that they packed satisfactorily in the unit. The rotation matrix between the two molecules of the asymmetric unit was determined and one molecule was used for the initial stages of model building.

E. Model building and crystallographic refinement

All subsequent refinement computing was done with the XPLOR program (Brunger et al (1987) Science 235, 458-460). 10% of the data were used for the calculation of R-free. To reduce model bias, partial models were used for map calculation and refinement. The initial partial model, containing a polyalanine chain of the secondary structure elements only, from the $\alpha 2$ I-domain structure, was subjected to conventional positional refinement and grouped B-factor refinement with strict non-crystallographic symmetry constraints.

The R and R-free factors dropped to 32.3% and 39.4% respectively. 3Fo -2Fc maps were used for cycles of model building and refinement. The resolution range used was from 8 to 3 Å. Typically, cycles consisted of model building, positional refinement and B-factor refinement. When the R and R-free reached 26% and 36% respectively, the 3 Å data set did not allow further improvement of the model. The 2.2 Å data set was collected at this point and was used for all subsequent model building and refinement. The R and R-free factors after the initial rigid body refinement at 2.2 Å were 41.3% and 42.2% respectively.

This larger data set allowed use of simulated annealing refinement and torsion angle dynamics refinement. As the phases improved, more atoms were added into the model. Initially, grouped B-factors were assigned for each residue (one for main chain and the one for side chain atoms). Later, non-crystallographic symmetry constraints were removed and individual atomic B-factors were refined for each residue. In addition bulk solvent correction was applied to the data set. Residues and side chains would be incorporated in the model if they were sufficiently well defined in 3Fo-2Fc electron density maps. Only manual structure modifications that resulted in lower R-free after refinement were accepted.

When R and R-free reached 29% and 34.8% respectively, water molecules were added by using the X-solvate utility of QUANTA. Finally, maximum likelihood refinement was used (Adams et al (1997) Proc.Nat.Acad.Sci USA 94, pp. 5018-5023) and resulted in the final structure with R and R-free of 23.5% and 30.2% respectively for data between 100 and 2.2 Å resolution. Table I summarizes information regarding crystallographic data and refinement. Table II lists the atomic coordinates of the I-domain of the $\alpha 1$ chain of the rat $\alpha 1\beta 1$ integrin. The coordinates of the crystal structure of the I-

domain may be used in the structure-based design of small molecule inhibitors of $\alpha 1\beta 1$, computational drug design and iterative structure optimization.

a. Computational drug design

Small molecule inhibitors can be designed using computational approaches. These approaches are also known as de novo drug design. In brief, the crystal structure coordinates of the $\alpha 1\beta 1$ integrin or fragment(s) thereof are the input for a computer program, such as DOCK. Programs such as DOCK output a list of small molecule structures that are expected to bind to $\alpha 1\beta 1$ or the fragment(s). These molecules can then be screened by biochemical assays for $\alpha 1\beta 1$ binding. Typically, biochemical assays that screen molecules for their ability to bind to $\alpha 1\beta 1$ or a fragment thereof are competition-type assays. In such assays, the molecule is added to the assay solution and the degree of inhibition is measured using conventional methodology.

An example of such an assay is the following: 96 well plates can be coated with collagen IV or collagen I and blocked with 3% Bovine Serum Albumin solution. Solution of $\alpha 1$ I-domain together with the small molecule under testing are incubated on the coated plates at room temperature for 1 hour and washed in triton buffer. Bound $\alpha 1$ I-domain is detected with a biotinylated anti-I-domain antibody. Plates are read at OD₄₀₅ on a microplate reader. The amount of bound I-domain is compared with a control experiment with no small molecule present. If it is lower than that of the control experiment that suggests inhibition by the small molecule.

b. Iterative cycles of structure optimization

The crystal structures of complexes formed between $\alpha 1\beta 1$ or a fragment and small molecule inhibitors may be solved. In brief, small molecule inhibitors are typically found using the crystal structure coordinates of a $\alpha 1\beta 1$ integrin or fragment either by the computational approaches mentioned above or by the screening of small molecule libraries. The small molecule inhibitor is then co-crystallized with $\alpha 1\beta 1$ or a fragment and the crystal structure of the complex is solved by molecular replacement. Molecular replacement requires the coordinates of a $\alpha 1\beta 1$ or fragment for the calculation of phases. The information collected from these experiments can be used to optimize the structure of small molecule inhibitors by clarifying how small molecules interact with the protein target. This suggests ways of modifying the small molecule to improve its

physicochemical properties, such as affinity, specificity, and kinetics with regard to the $\alpha 1\beta 1$ target.

In addition to being necessary for computational drug design and structure optimization, the crystal coordinates described herein are useful for analyzing the $\alpha 1\beta 1$ binding site. Through such analysis, it was determined that a particularly attractive region for drug targeting is in the vicinity of residues Asp154, Ser156, Asn157, Ser158, Leu222, Gln223, Thr224, Asp257, Glu259, His261, His288, Tyr289, Gly292, Leu294 and Lys298. The above observations and hypotheses suggest that this region may contribute significantly to the binding energy of $\alpha 1\beta 1$ /ECM interactions, and therefore, is an attractive target for inhibitor design. Site mutations studies can be used in conjunction with the above-described processes to further define the binding site.

It will be apparent to those skilled in the art that various modifications and variations can be made in the methods and compositions of the present invention without departing from the spirit or scope of the invention. Thus, it is intended that the present invention cover the modifications and variations of this invention provided that they come within the scope of the appended claims and their equivalents.

TABLE I: Crystallographic data statistics:

Symmetry:	P2 ₁ 2 ₁ 2 ₁
Unit cell (Å)	a = 34.77, b = 85.92, c = 132.56
No.of crystals:	1
Resolution (Å)	2.2
Reflections(unique):	19,238
R _{merge}	5.6%
Completeness:	91.3%
Completeness(2.2-2.28 Å)	77.6%

TABLE II: Crystallographic coordinates of the alpha1 I-domain crystal structure in PDB(XPLOR) format.

Segment names A, B, W correspond to molecule A, molecule B and water respectively.

CRYST	34.770	85.920	132.560	90.00	90.00	90.00	P212121	
ATOM	1	CB	ALA	145	35.261	87.828	-14.480	1.00 46.82 A
ATOM	2	C	ALA	145	33.051	87.078	-15.373	1.00 48.98 A
ATOM	3	O	ALA	145	32.414	87.150	-14.310	1.00 49.22 A
ATOM	4	HT1	ALA	145	33.390	89.717	-14.876	1.00 0.00 A
ATOM	5	HT2	ALA	145	33.206	89.509	-16.551	1.00 0.00 A
ATOM	6	N	ALA	145	33.860	89.407	-15.751	1.00 47.03 A
ATOM	7	HT3	ALA	145	34.705	89.992	-15.916	1.00 0.00 A
ATOM	8	CA	ALA	145	34.266	87.977	-15.619	1.00 46.67 A

5	ATOM	9	N	ALA	146	32.737	86.234	-16.358	1.00	42.12	A
	ATOM	10	H	ALA	146	33.287	86.229	-17.170	1.00	0.00	A
	ATOM	11	CA	ALA	146	31.603	85.321	-16.264	1.00	40.10	A
	ATOM	12	CB	ALA	146	31.657	84.314	-17.389	1.00	35.92	A
	ATOM	13	C	ALA	146	31.621	84.602	-14.919	1.00	40.80	A
10	ATOM	14	O	ALA	146	32.511	83.799	-14.647	1.00	42.91	A
	ATOM	15	N	LEU	147	30.629	84.888	-14.082	1.00	37.99	A
	ATOM	16	H	LEU	147	29.931	85.517	-14.359	1.00	0.00	A
	ATOM	17	CA	LEU	147	30.562	84.284	-12.759	1.00	37.93	A
	ATOM	18	CB	LEU	147	31.411	85.107	-11.803	1.00	38.26	A
15	ATOM	19	CG	LEU	147	31.994	84.349	-10.623	1.00	39.33	A
	ATOM	20	CD1	LEU	147	33.183	83.510	-11.078	1.00	33.15	A
	ATOM	21	CD2	LEU	147	32.389	85.347	-9.567	1.00	38.31	A
	ATOM	22	C	LEU	147	29.156	84.164	-12.181	1.00	36.60	A
	ATOM	23	O	LEU	147	28.417	85.142	-12.132	1.00	37.06	A
20	ATOM	24	N	ASP	148	28.780	82.966	-11.751	1.00	36.31	A
	ATOM	25	H	ASP	148	29.384	82.200	-11.844	1.00	0.00	A
	ATOM	26	CA	ASP	148	27.468	82.788	-11.140	1.00	33.40	A
	ATOM	27	CB	ASP	148	26.836	81.461	-11.589	1.00	35.41	A
	ATOM	28	CG	ASP	148	26.085	81.583	-12.925	1.00	33.40	A
25	ATOM	29	OD1	ASP	148	25.783	80.537	-13.531	1.00	32.84	A
	ATOM	30	OD2	ASP	148	25.795	82.715	-13.376	1.00	33.54	A
	ATOM	31	C	ASP	148	27.695	82.829	-9.622	1.00	28.37	A
	ATOM	32	O	ASP	148	28.475	82.050	-9.070	1.00	26.95	A
	ATOM	33	N	ILE	149	27.027	83.767	-8.961	1.00	25.21	A
30	ATOM	34	H	ILE	149	26.411	84.349	-9.453	1.00	0.00	A
	ATOM	35	CA	ILE	149	27.179	83.957	-7.529	1.00	24.78	A
	ATOM	36	CB	ILE	149	27.883	85.308	-7.229	1.00	25.55	A
	ATOM	37	CG2	ILE	149	28.047	85.509	-5.718	1.00	19.80	A
	ATOM	38	CG1	ILE	149	29.233	85.363	-7.947	1.00	21.46	A
35	ATOM	39	CD1	ILE	149	29.730	86.775	-8.168	1.00	25.74	A
	ATOM	40	C	ILE	149	25.853	83.957	-6.786	1.00	27.12	A
	ATOM	41	O	ILE	149	24.957	84.737	-7.097	1.00	27.87	A
	ATOM	42	N	VAL	150	25.748	83.101	-5.780	1.00	29.44	A
	ATOM	43	H	VAL	150	26.498	82.509	-5.564	1.00	0.00	A
40	ATOM	44	CA	VAL	150	24.525	83.031	-4.990	1.00	31.56	A
	ATOM	45	CB	VAL	150	23.914	81.612	-5.015	1.00	33.68	A
	ATOM	46	CG1	VAL	150	22.921	81.433	-3.871	1.00	36.22	A
	ATOM	47	CG2	VAL	150	23.218	81.387	-6.339	1.00	35.65	A
	ATOM	48	C	VAL	150	24.751	83.443	-3.543	1.00	29.32	A
45	ATOM	49	O	VAL	150	25.643	82.939	-2.849	1.00	27.25	A
	ATOM	50	N	ILE	151	23.936	84.383	-3.096	1.00	29.18	A
	ATOM	51	H	ILE	151	23.269	84.772	-3.699	1.00	0.00	A
	ATOM	52	CA	ILE	151	24.016	84.847	-1.724	1.00	28.46	A
	ATOM	53	CB	ILE	151	23.614	86.340	-1.625	1.00	27.62	A
50	ATOM	54	CG2	ILE	151	23.843	86.860	-0.209	1.00	24.70	A
	ATOM	55	CG1	ILE	151	24.457	87.167	-2.607	1.00	27.55	A
	ATOM	56	CD1	ILE	151	23.788	87.443	-3.933	1.00	28.07	A
	ATOM	57	C	ILE	151	23.067	83.964	-0.908	1.00	26.00	A
	ATOM	58	O	ILE	151	21.923	83.721	-1.307	1.00	25.72	A
55	ATOM	59	N	VAL	152	23.575	83.445	0.199	1.00	22.21	A
	ATOM	60	H	VAL	152	24.506	83.650	0.427	1.00	0.00	A
	ATOM	61	CA	VAL	152	22.813	82.581	1.099	1.00	23.05	A
	ATOM	62	CB	VAL	152	23.585	81.247	1.402	1.00	26.59	A
	ATOM	63	CG1	VAL	152	22.665	80.246	2.127	1.00	25.59	A
60	ATOM	64	CG2	VAL	152	24.102	80.628	0.094	1.00	21.54	A
	ATOM	65	C	VAL	152	22.689	83.412	2.366	1.00	20.44	A
	ATOM	66	O	VAL	152	23.554	83.369	3.246	1.00	14.87	A
	ATOM	67	N	LEU	153	21.613	84.180	2.442	1.00	20.46	A
	ATOM	68	H	LEU	153	20.950	84.144	1.721	1.00	0.00	A
65	ATOM	69	CA	LEU	153	21.384	85.071	3.563	1.00	19.62	A
	ATOM	70	CB	LEU	153	20.780	86.370	3.044	1.00	27.82	A
	ATOM	71	CG	LEU	153	20.357	87.482	4.001	1.00	29.39	A
	ATOM	72	CD1	LEU	153	21.555	88.057	4.739	1.00	32.60	A
	ATOM	73	CD2	LEU	153	19.683	88.565	3.170	1.00	34.32	A
70	ATOM	74	C	LEU	153	20.518	84.490	4.659	1.00	22.92	A
	ATOM	75	O	LEU	153	19.360	84.122	4.445	1.00	20.87	A
	ATOM	76	N	ASP	154	21.101	84.430	5.846	1.00	20.52	A
	ATOM	77	H	ASP	154	22.026	84.747	5.930	1.00	0.00	A
	ATOM	78	CA	ASP	154	20.439	83.917	7.020	1.00	20.46	A
	ATOM	79	CB	ASP	154	21.506	83.624	8.078	1.00	22.44	A
	ATOM	80	CG	ASP	154	20.946	83.418	9.462	1.00	20.33	A
	ATOM	81	OD1	ASP	154	19.773	83.017	9.617	1.00	25.28	A

	ATOM	82	OD2	ASP	154	21.709	83.658	10.408	1.00	17.38	A
	ATOM	83	C	ASP	154	19.463	85.012	7.445	1.00	24.81	A
	ATOM	84	O	ASP	154	19.850	86.170	7.680	1.00	19.94	A
5	ATOM	85	N	GLY	155	18.186	84.645	7.491	1.00	22.66	A
	ATOM	86	H	GLY	155	17.945	83.724	7.270	1.00	0.00	A
	ATOM	87	CA	GLY	155	17.154	85.583	7.865	1.00	25.80	A
	ATOM	88	C	GLY	155	16.573	85.333	9.242	1.00	27.90	A
	ATOM	89	O	GLY	155	15.411	85.623	9.465	1.00	30.07	A
10	ATOM	90	N	SER	156	17.363	84.783	10.158	1.00	29.73	A
	ATOM	91	H	SER	156	18.280	84.539	9.917	1.00	0.00	A
	ATOM	92	CA	SER	156	16.887	84.533	11.519	1.00	33.03	A
	ATOM	93	CB	SER	156	17.956	83.778	12.327	1.00	33.06	A
	ATOM	94	OG	SER	156	18.696	84.658	13.163	1.00	34.46	A
15	ATOM	95	HG	SER	156	19.354	84.158	13.652	1.00	0.00	A
	ATOM	96	C	SER	156	16.589	85.896	12.162	1.00	28.30	A
	ATOM	97	O	SER	156	16.928	86.935	11.595	1.00	32.92	A
	ATOM	98	N	ASN	157	15.958	85.892	13.335	1.00	27.00	A
	ATOM	99	H	ASN	157	15.732	85.033	13.746	1.00	0.00	A
20	ATOM	100	CA	ASN	157	15.591	87.140	14.032	1.00	22.66	A
	ATOM	101	CB	ASN	157	14.545	86.871	15.127	1.00	24.65	A
	ATOM	102	CG	ASN	157	13.322	86.095	14.644	1.00	26.95	A
	ATOM	103	OD1	ASN	157	12.722	85.354	15.422	1.00	22.76	A
	ATOM	104	ND2	ASN	157	12.941	86.269	13.380	1.00	23.43	A
25	ATOM	105	HD21	ASN	157	13.442	86.879	12.800	1.00	0.00	A
	ATOM	106	HD22	ASN	157	12.156	85.772	13.074	1.00	0.00	A
	ATOM	107	C	ASN	157	16.724	87.922	14.717	1.00	20.73	A
	ATOM	108	O	ASN	157	16.488	89.024	15.179	1.00	19.35	A
	ATOM	109	N	SER	158	17.936	87.382	14.804	1.00	20.15	A
30	ATOM	110	H	SER	158	18.117	86.511	14.395	1.00	0.00	A
	ATOM	111	CA	SER	158	19.005	88.099	15.519	1.00	17.25	A
	ATOM	112	CB	SER	158	20.003	87.095	16.115	1.00	18.79	A
	ATOM	113	OG	SER	158	20.309	86.048	15.204	1.00	21.49	A
	ATOM	114	HG	SER	158	20.692	86.418	14.407	1.00	0.00	A
35	ATOM	115	C	SER	158	19.764	89.191	14.750	1.00	19.11	A
	ATOM	116	O	SER	158	20.168	90.196	15.331	1.00	15.49	A
	ATOM	117	N	ILE	159	19.985	88.994	13.462	1.00	19.24	A
	ATOM	118	H	ILE	159	19.683	88.164	13.037	1.00	0.00	A
40	ATOM	119	CA	ILE	159	20.674	90.002	12.670	1.00	24.70	A
	ATOM	120	CB	ILE	159	20.702	89.596	11.193	1.00	25.84	A
	ATOM	121	CG2	ILE	159	21.185	90.750	10.347	1.00	23.12	A
	ATOM	122	CG1	ILE	159	21.602	88.366	11.029	1.00	30.68	A
	ATOM	123	CD1	ILE	159	21.058	87.313	10.092	1.00	36.48	A
	ATOM	124	C	ILE	159	19.755	91.188	12.863	1.00	29.72	A
45	ATOM	125	O	ILE	159	18.733	91.293	12.201	1.00	27.59	A
	ATOM	126	N	TYR	160	20.099	92.098	13.764	1.00	32.64	A
	ATOM	127	H	TYR	160	20.953	92.057	14.240	1.00	0.00	A
	ATOM	128	CA	TYR	160	19.142	93.153	13.995	1.00	36.31	A
	ATOM	129	CB	TYR	160	19.262	93.759	15.384	1.00	29.60	A
50	ATOM	130	CG	TYR	160	18.250	94.871	15.541	1.00	25.36	A
	ATOM	131	CD1	TYR	160	16.953	94.731	15.034	1.00	30.44	A
	ATOM	132	CE1	TYR	160	16.027	95.768	15.113	1.00	28.80	A
	ATOM	133	CD2	TYR	160	18.597	96.077	16.131	1.00	22.43	A
	ATOM	134	CE2	TYR	160	17.686	97.118	16.218	1.00	29.79	A
55	ATOM	135	CZ	TYR	160	16.406	96.958	15.706	1.00	29.67	A
	ATOM	136	OH	TYR	160	15.514	97.989	15.801	1.00	35.06	A
	ATOM	137	HH	TYR	160	14.682	97.730	15.399	1.00	0.00	A
	ATOM	138	C	TYR	160	19.015	94.279	13.018	1.00	38.57	A
	ATOM	139	O	TYR	160	18.019	94.342	12.297	1.00	45.05	A
60	ATOM	140	N	PRO	161	19.992	95.194	12.969	1.00	34.46	A
	ATOM	141	CD	PRO	161	21.298	95.354	13.624	1.00	23.12	A
	ATOM	142	CA	PRO	161	19.727	96.237	11.978	1.00	32.11	A
	ATOM	143	CB	PRO	161	20.946	97.155	12.068	1.00	30.05	A
	ATOM	144	CG	PRO	161	21.657	96.769	13.287	1.00	34.00	A
65	ATOM	145	C	PRO	161	19.578	95.579	10.605	1.00	30.24	A
	ATOM	146	O	PRO	161	20.555	95.434	9.878	1.00	29.38	A
	ATOM	147	N	TRP	162	18.365	95.167	10.254	1.00	28.87	A
	ATOM	148	H	TRP	162	17.603	95.296	10.855	1.00	0.00	A
	ATOM	149	CA	TRP	162	18.180	94.525	8.970	1.00	29.54	A
70	ATOM	150	CB	TRP	162	16.725	94.114	8.744	1.00	28.05	A
	ATOM	151	CG	TRP	162	16.577	93.324	7.456	1.00	27.54	A
	ATOM	152	CD2	TRP	162	17.115	92.017	7.176	1.00	22.18	A
	ATOM	153	CE2	TRP	162	16.795	91.710	5.837	1.00	27.60	A
	ATOM	154	CE3	TRP	162	17.831	91.081	7.935	1.00	22.75	A

	ATOM	155	CD1	TRP	162	15.976	93.740	6.304	1.00	27.18	A
	ATOM	156	NE1	TRP	162	16.103	92.779	5.324	1.00	31.45	A
	ATOM	157	HE1	TRP	162	15.756	92.847	4.416	1.00	0.00	A
5	ATOM	158	CZ2	TRP	162	17.169	90.503	5.230	1.00	25.17	A
	ATOM	159	CZ3	TRP	162	18.201	89.879	7.343	1.00	21.51	A
	ATOM	160	CH2	TRP	162	17.872	89.601	5.998	1.00	27.23	A
	ATOM	161	C	TRP	162	18.644	95.419	7.825	1.00	32.23	A
	ATOM	162	O	TRP	162	19.318	94.945	6.914	1.00	29.79	A
10	ATOM	163	N	GLU	163	18.314	96.708	7.859	1.00	34.04	A
	ATOM	164	H	GLU	163	17.794	97.072	8.607	1.00	0.00	A
	ATOM	165	CA	GLU	163	18.744	97.572	6.757	1.00	36.74	A
	ATOM	166	CB	GLU	163	18.235	99.011	6.936	1.00	33.42	A
	ATOM	167	CG	GLU	163	17.941	99.437	8.355	1.00	41.87	A
	ATOM	168	CD	GLU	163	18.085	100.938	8.529	1.00	43.51	A
15	ATOM	169	OE1	GLU	163	19.238	101.426	8.588	1.00	44.11	A
	ATOM	170	OE2	GLU	163	17.047	101.629	8.597	1.00	39.73	A
	ATOM	171	C	GLU	163	20.267	97.578	6.566	1.00	35.78	A
	ATOM	172	O	GLU	163	20.769	98.002	5.519	1.00	29.20	A
20	ATOM	173	N	SER	164	20.987	97.083	7.574	1.00	35.57	A
	ATOM	174	H	SER	164	20.516	96.748	8.364	1.00	0.00	A
	ATOM	175	CA	SER	164	22.443	97.024	7.547	1.00	31.38	A
	ATOM	176	CB	SER	164	22.990	96.956	8.968	1.00	30.80	A
	ATOM	177	OG	SER	164	22.876	98.211	9.605	1.00	37.22	A
	ATOM	178	HG	SER	164	23.225	98.151	10.498	1.00	0.00	A
25	ATOM	179	C	SER	164	22.964	95.837	6.751	1.00	32.24	A
	ATOM	180	O	SER	164	24.084	95.870	6.231	1.00	37.08	A
	ATOM	181	N	VAL	165	22.171	94.775	6.688	1.00	31.62	A
	ATOM	182	H	VAL	165	21.316	94.783	7.165	1.00	0.00	A
30	ATOM	183	CA	VAL	165	22.553	93.602	5.916	1.00	31.01	A
	ATOM	184	CB	VAL	165	21.623	92.401	6.164	1.00	35.77	A
	ATOM	185	CG1	VAL	165	22.339	91.110	5.787	1.00	39.39	A
	ATOM	186	CG2	VAL	165	21.177	92.366	7.607	1.00	40.80	A
	ATOM	187	C	VAL	165	22.328	94.049	4.493	1.00	32.48	A
35	ATOM	188	O	VAL	165	23.156	93.824	3.609	1.00	35.34	A
	ATOM	189	N	ILE	166	21.187	94.701	4.297	1.00	33.35	A
	ATOM	190	H	ILE	166	20.586	94.837	5.058	1.00	0.00	A
	ATOM	191	CA	ILE	166	20.789	95.225	2.997	1.00	32.78	A
	ATOM	192	CB	ILE	166	19.382	95.862	3.078	1.00	31.47	A
40	ATOM	193	CG2	ILE	166	19.056	96.575	1.783	1.00	32.21	A
	ATOM	194	CG1	ILE	166	18.346	94.785	3.419	1.00	30.98	A
	ATOM	195	CD1	ILE	166	16.917	95.142	3.048	1.00	25.05	A
	ATOM	196	C	ILE	166	21.800	96.267	2.504	1.00	30.96	A
	ATOM	197	O	ILE	166	22.159	96.293	1.326	1.00	31.98	A
45	ATOM	198	N	ALA	167	22.260	97.120	3.410	1.00	31.52	A
	ATOM	199	H	ALA	167	21.947	97.057	4.337	1.00	0.00	A
	ATOM	200	CA	ALA	167	23.228	98.153	3.047	1.00	33.64	A
	ATOM	201	CB	ALA	167	23.540	99.023	4.253	1.00	29.88	A
	ATOM	202	C	ALA	167	24.502	97.482	2.539	1.00	35.05	A
50	ATOM	203	O	ALA	167	25.176	97.982	1.630	1.00	30.30	A
	ATOM	204	N	PHE	168	24.821	96.342	3.141	1.00	31.11	A
	ATOM	205	H	PHE	168	24.245	96.013	3.864	1.00	0.00	A
	ATOM	206	CA	PHE	168	25.987	95.572	2.771	1.00	28.96	A
	ATOM	207	CB	PHE	168	26.214	94.504	3.835	1.00	32.92	A
55	ATOM	208	CG	PHE	168	27.007	93.329	3.371	1.00	29.30	A
	ATOM	209	CD1	PHE	168	26.378	92.118	3.111	1.00	31.94	A
	ATOM	210	CD2	PHE	168	28.386	93.405	3.266	1.00	26.68	A
	ATOM	211	CE1	PHE	168	27.104	90.990	2.760	1.00	28.37	A
	ATOM	212	CE2	PHE	168	29.128	92.282	2.913	1.00	31.48	A
60	ATOM	213	CZ	PHE	168	28.481	91.071	2.660	1.00	33.94	A
	ATOM	214	C	PHE	168	25.736	94.955	1.395	1.00	30.36	A
	ATOM	215	O	PHE	168	26.549	95.106	0.482	1.00	25.57	A
	ATOM	216	N	LEU	169	24.602	94.279	1.241	1.00	29.42	A
	ATOM	217	H	LEU	169	23.985	94.192	1.997	1.00	0.00	A
65	ATOM	218	CA	LEU	169	24.262	93.666	-0.037	1.00	32.92	A
	ATOM	219	CB	LEU	169	22.835	93.109	-0.008	1.00	30.46	A
	ATOM	220	CG	LEU	169	22.485	91.838	0.773	1.00	27.73	A
	ATOM	221	CD1	LEU	169	21.107	91.386	0.309	1.00	23.84	A
	ATOM	222	CD2	LEU	169	23.504	90.738	0.549	1.00	22.89	A
70	ATOM	223	C	LEU	169	24.371	94.717	-1.148	1.00	36.13	A
	ATOM	224	O	LEU	169	24.992	94.484	-2.181	1.00	37.86	A
	ATOM	225	N	ASN	170	23.760	95.876	-0.920	1.00	39.95	A
	ATOM	226	H	ASN	170	23.279	95.996	-0.078	1.00	0.00	A
	ATOM	227	CA	ASN	170	23.779	96.977	-1.882	1.00	35.60	A

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5	ATOM	228	CB	ASN	170	23.040	98.179	-1.275	1.00	40.87	A
	ATOM	229	CG	ASN	170	23.122	99.427	-2.140	1.00	45.43	A
	ATOM	230	OD1	ASN	170	24.008	100.268	-1.958	1.00	38.53	A
	ATOM	231	ND2	ASN	170	22.191	99.558	-3.083	1.00	44.25	A
	ATOM	232	HD21	ASN	170	21.503	98.868	-3.188	1.00	0.00	A
10	ATOM	233	HD22	ASN	170	22.229	100.355	-3.648	1.00	0.00	A
	ATOM	234	C	ASN	170	25.221	97.354	-2.203	1.00	37.08	A
	ATOM	235	O	ASN	170	25.590	97.546	-3.360	1.00	36.45	A
	ATOM	236	N	ASP	171	26.022	97.444	-1.149	1.00	41.63	A
	ATOM	237	H	ASP	171	25.640	97.256	-0.267	1.00	0.00	A
15	ATOM	238	CA	ASP	171	27.430	97.805	-1.219	1.00	45.96	A
	ATOM	239	CB	ASP	171	27.984	97.921	0.205	1.00	49.80	A
	ATOM	240	CG	ASP	171	28.976	99.051	0.360	1.00	58.06	A
	ATOM	241	OD1	ASP	171	28.606	100.218	0.111	1.00	61.54	A
	ATOM	242	OD2	ASP	171	30.131	98.771	0.738	1.00	60.67	A
20	ATOM	243	C	ASP	171	28.286	96.815	-2.018	1.00	47.51	A
	ATOM	244	O	ASP	171	29.263	97.214	-2.656	1.00	45.54	A
	ATOM	245	N	LEU	172	27.923	95.535	-1.972	1.00	44.73	A
	ATOM	246	H	LEU	172	27.131	95.289	-1.448	1.00	0.00	A
	ATOM	247	CA	LEU	172	28.658	94.480	-2.675	1.00	43.36	A
25	ATOM	248	CB	LEU	172	28.434	93.125	-1.985	1.00	37.47	A
	ATOM	249	CG	LEU	172	29.574	92.102	-1.869	1.00	35.42	A
	ATOM	250	CD1	LEU	172	29.011	90.764	-1.398	1.00	32.59	A
	ATOM	251	CD2	LEU	172	30.274	91.926	-3.189	1.00	32.89	A
	ATOM	252	C	LEU	172	28.214	94.362	-4.122	1.00	43.76	A
30	ATOM	253	O	LEU	172	29.013	94.070	-5.011	1.00	42.82	A
	ATOM	254	N	LEU	173	26.928	94.587	-4.345	1.00	45.41	A
	ATOM	255	H	LEU	173	26.349	94.834	-3.595	1.00	0.00	A
	ATOM	256	CA	LEU	173	26.354	94.481	-5.674	1.00	49.41	A
	ATOM	257	CB	LEU	173	24.837	94.308	-5.561	1.00	52.76	A
35	ATOM	258	CG	LEU	173	24.329	92.938	-5.089	1.00	54.19	A
	ATOM	259	CD1	LEU	173	24.148	92.038	-6.294	1.00	59.26	A
	ATOM	260	CD2	LEU	173	25.302	92.305	-4.110	1.00	54.13	A
	ATOM	261	C	LEU	173	26.681	95.681	-6.552	1.00	51.49	A
	ATOM	262	O	LEU	173	27.079	95.521	-7.708	1.00	46.63	A
40	ATOM	263	N	LYS	174	26.523	96.882	-5.997	1.00	51.16	A
	ATOM	264	H	LYS	174	26.220	96.946	-5.068	1.00	0.00	A
	ATOM	265	CA	LYS	174	26.794	98.096	-6.751	1.00	51.25	A
	ATOM	266	CB	LYS	174	26.615	99.330	-5.862	1.00	50.79	A
	ATOM	267	CG	LYS	174	27.294	99.251	-4.513	1.00	49.59	A
45	ATOM	268	CD	LYS	174	26.659	100.247	-3.542	1.00	48.26	A
	ATOM	269	CE	LYS	174	27.707	100.970	-2.714	1.00	41.18	A
	ATOM	270	NZ	LYS	174						

5	ATOM	301	O	MET	176	28.361	95.542	-11.049	1.00	46.58	A
	ATOM	302	N	ASP	177	29.656	94.035	-12.118	1.00	51.49	A
	ATOM	303	H	ASP	177	30.352	93.353	-12.016	1.00	0.00	A
	ATOM	304	CA	ASP	177	29.157	94.329	-13.457	1.00	54.36	A
	ATOM	305	CB	ASP	177	30.322	94.519	-14.441	1.00	56.10	A
	ATOM	306	CG	ASP	177	30.746	95.974	-14.586	1.00	60.14	A
	ATOM	307	OD1	ASP	177	31.960	96.219	-14.732	1.00	58.72	A
10	ATOM	308	OD2	ASP	177	29.874	96.868	-14.559	1.00	61.23	A
	ATOM	309	C	ASP	177	28.366	93.070	-13.833	1.00	54.37	A
	ATOM	310	O	ASP	177	28.944	92.089	-14.304	1.00	54.71	A
	ATOM	311	N	ILE	178	27.056	93.088	-13.603	1.00	50.87	A
15	ATOM	312	H	ILE	178	26.644	93.892	-13.226	1.00	0.00	A
	ATOM	313	CA	ILE	178	26.220	91.929	-13.905	1.00	50.24	A
	ATOM	314	CB	ILE	178	24.921	91.933	-13.041	1.00	49.66	A
	ATOM	315	CG2	ILE	178	24.214	90.581	-13.131	1.00	49.10	A
	ATOM	316	CG1	ILE	178	25.275	92.217	-11.576	1.00	50.99	A
20	ATOM	317	CD1	ILE	178	24.125	92.001	-10.593	1.00	52.23	A
	ATOM	318	C	ILE	178	25.855	91.871	-15.386	1.00	48.57	A
	ATOM	319	O	ILE	178	25.743	92.905	-16.040	1.00	50.81	A
	ATOM	320	N	GLY	179	25.689	90.654	-15.902	1.00	48.26	A
	ATOM	321	H	GLY	179	25.801	89.873	-15.324	1.00	0.00	A
25	ATOM	322	CA	GLY	179	25.341	90.453	-17.300	1.00	47.18	A
	ATOM	323	C	GLY	179	25.483	88.993	-17.708	1.00	47.42	A
	ATOM	324	O	GLY	179	26.366	88.302	-17.203	1.00	44.46	A
	ATOM	325	N	PRO	180	24.635	88.489	-18.621	1.00	48.62	A
	ATOM	326	CD	PRO	180	23.543	89.194	-19.313	1.00	50.81	A
30	ATOM	327	CA	PRO	180	24.730	87.084	-19.046	1.00	49.53	A
	ATOM	328	CB	PRO	180	23.635	86.946	-20.107	1.00	48.70	A
	ATOM	329	CG	PRO	180	22.692	88.070	-19.837	1.00	52.71	A
	ATOM	330	C	PRO	180	26.104	86.712	-19.597	1.00	52.68	A
	ATOM	331	O	PRO	180	26.359	85.541	-19.902	1.00	53.20	A
35	ATOM	332	N	LYS	181	26.983	87.706	-19.716	1.00	49.61	A
	ATOM	333	H	LYS	181	26.720	88.610	-19.445	1.00	0.00	A
	ATOM	334	CA	LYS	181	28.324	87.485	-20.238	1.00	49.94	A
	ATOM	335	CB	LYS	181	28.517	88.279	-21.535	1.00	52.40	A
	ATOM	336	CG	LYS	181	27.413	88.064	-22.577	1.00	52.89	A
40	ATOM	337	CD	LYS	181	27.111	86.588	-22.801	1.00	50.48	A
	ATOM	338	CE	LYS	181	28.125	85.942	-23.735	1.00	54.32	A
	ATOM	339	NZ	LYS	181	29.156	85.176	-22.981	1.00	54.02	A
	ATOM	340	HZ1	LYS	181	28.696	84.425	-22.427	1.00	0.00	A
	ATOM	341	HZ2	LYS	181	29.664	85.818	-22.338	1.00	0.00	A
45	ATOM	342	HZ3	LYS	181	29.830	84.750	-23.648	1.00	0.00	A
	ATOM	343									

	ATOM	374	HE21	GLN	184	23.400	86.330	-16.503	1.00	0.00	A
	ATOM	375	HE22	GLN	184	22.470	84.910	-16.770	1.00	0.00	A
	ATOM	376	C	GLN	184	24.956	86.687	-11.032	1.00	34.89	A
	ATOM	377	O	GLN	184	25.816	86.138	-10.331	1.00	31.60	A
5	ATOM	378	N	VAL	185	23.819	87.185	-10.552	1.00	35.52	A
	ATOM	379	H	VAL	185	23.168	87.567	-11.175	1.00	0.00	A
	ATOM	380	CA	VAL	185	23.510	87.179	-9.129	1.00	33.81	A
	ATOM	381	CB	VAL	185	23.602	88.617	-8.545	1.00	35.05	A
10	ATOM	382	CG1	VAL	185	23.088	88.636	-7.094	1.00	35.71	A
	ATOM	383	CG2	VAL	185	25.048	89.115	-8.612	1.00	16.86	A
	ATOM	384	C	VAL	185	22.137	86.604	-8.772	1.00	34.96	A
	ATOM	385	O	VAL	185	21.129	86.859	-9.441	1.00	29.48	A
	ATOM	386	N	GLY	186	22.129	85.830	-7.691	1.00	29.37	A
	ATOM	387	H	GLY	186	22.968	85.675	-7.209	1.00	0.00	A
15	ATOM	388	CA	GLY	186	20.915	85.215	-7.208	1.00	33.55	A
	ATOM	389	C	GLY	186	20.922	85.345	-5.706	1.00	30.62	A
	ATOM	390	O	GLY	186	21.978	85.507	-5.092	1.00	38.55	A
	ATOM	391	N	ILE	187	19.751	85.285	-5.100	1.00	29.16	A
	ATOM	392	H	ILE	187	18.935	85.152	-5.626	1.00	0.00	A
20	ATOM	393	CA	ILE	187	19.667	85.411	-3.657	1.00	29.27	A
	ATOM	394	CB	ILE	187	19.244	86.832	-3.222	1.00	23.80	A
	ATOM	395	CG2	ILE	187	19.187	86.902	-1.708	1.00	21.78	A
	ATOM	396	CG1	ILE	187	20.223	87.869	-3.771	1.00	25.79	A
	ATOM	397	CD1	ILE	187	20.020	89.264	-3.200	1.00	26.87	A
25	ATOM	398	C	ILE	187	18.656	84.456	-3.063	1.00	28.09	A
	ATOM	399	O	ILE	187	17.537	84.337	-3.549	1.00	26.92	A
	ATOM	400	N	VAL	188	19.057	83.793	-1.989	1.00	31.92	A
	ATOM	401	H	VAL	188	19.971	83.924	-1.660	1.00	0.00	A
	ATOM	402	CA	VAL	188	18.175	82.877	-1.288	1.00	31.88	A
30	ATOM	403	CB	VAL	188	18.598	81.408	-1.538	1.00	30.39	A
	ATOM	404	CG1	VAL	188	18.918	80.702	-0.221	1.00	23.72	A
	ATOM	405	CG2	VAL	188	17.478	80.688	-2.276	1.00	31.57	A
	ATOM	406	C	VAL	188	18.271	83.226	0.198	1.00	30.17	A
	ATOM	407	O	VAL	188	19.362	83.436	0.719	1.00	29.85	A
35	ATOM	408	N	GLN	189	17.132	83.332	0.869	1.00	26.31	A
	ATOM	409	H	GLN	189	16.278	83.201	0.405	1.00	0.00	A
	ATOM	410	CA	GLN	189	17.146	83.644	2.288	1.00	27.42	A
	ATOM	411	CB	GLN	189	16.219	84.830	2.629	1.00	25.02	A
	ATOM	412	CG	GLN	189	16.196	85.140	4.141	1.00	21.62	A
40	ATOM	413	CD	GLN	189	15.631	86.506	4.495	1.00	22.57	A
	ATOM	414	OE1	GLN	189	15.554	86.867	5.668	1.00	23.48	A
	ATOM	415	NE2	GLN	189	15.230	87.263	3.487	1.00	26.01	A
	ATOM	416	HE21	GLN	189	15.304	86.940	2.567	1.00	0.00	A
	ATOM	417	HE22	GLN	189	14.866	88.147	3.709	1.00	0.00	A
45	ATOM	418	C	GLN	189	16.679	82.392	3.000	1.00	23.00	A
	ATOM	419	O	GLN	189	15.882	81.631	2.463	1.00	23.43	A
	ATOM	420	N	TYR	190	17.184	82.171	4.202	1.00	22.53	A
	ATOM	421	H	TYR	190	17.820	82.811	4.584	1.00	0.00	A
	ATOM	422	CA	TYR	190	16.811	80.993	4.963	1.00	26.52	A
50	ATOM	423	CB	TYR	190	17.837	79.883	4.726	1.00	26.90	A
	ATOM	424	CG	TYR	190	19.147	80.113	5.453	1.00	17.55	A
	ATOM	425	CD1	TYR	190	19.397	79.503	6.676	1.00	15.45	A
	ATOM	426	CE1	TYR	190	20.593	79.699	7.345	1.00	17.09	A
	ATOM	427	CD2	TYR	190	20.139	80.936	4.907	1.00	14.28	A
55	ATOM	428	CE2	TYR	190	21.347	81.138	5.568	1.00	14.48	A
	ATOM	429	CZ	TYR	190	21.567	80.513	6.786	1.00	15.88	A
	ATOM	430	OH	TYR	190	22.749	80.701	7.467	1.00	15.41	A
	ATOM	431	HH	TYR	190	23.313	81.297	6.966	1.00	0.00	A
	ATOM	432	C	TYR	190	16.694	81.265	6.463	1.00	28.88	A
60	ATOM	433	O	TYR	190	17.147	82.297	6.974	1.00	27.66	A
	ATOM	434	N	GLY	191	16.093	80.302	7.152	1.00	29.28	A
	ATOM	435	H	GLY	191	15.773	79.511	6.669	1.00	0.00	A
	ATOM	436	CA	GLY	191	15.888	80.359	8.587	1.00	26.48	A
	ATOM	437	C	GLY	191	14.655	79.507	8.787	1.00	27.88	A
65	ATOM	438	O	GLY	191	13.548	79.953	8.494	1.00	33.37	A
	ATOM	439	N	GLU	192	14.843	78.283	9.266	1.00	31.94	A
	ATOM	440	H	GLU	192	15.753	78.004	9.499	1.00	0.00	A
	ATOM	441	CA	GLU	192	13.744	77.334	9.461	1.00	34.41	A
	ATOM	442	CB	GLU	192	12.504	78.026	10.025	1.00	39.00	A
70	ATOM	443	CG	GLU	192	12.439	78.147	11.534	1.00	39.53	A
	ATOM	444	CD	GLU	192	11.319	79.079	11.967	1.00	39.25	A
	ATOM	445	OE1	GLU	192	11.611	80.085	12.645	1.00	42.52	A
	ATOM	446	OE2	GLU	192	10.146	78.813	11.616	1.00	34.89	A

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	ATOM	447	C	GLU	192	13.384	76.697	8.111	1.00	34.47	A
	ATOM	448	O	GLU	192	13.208	75.487	8.010	1.00	36.09	A
	ATOM	449	N	ASN	193	13.265	77.528	7.082	1.00	33.33	A
	ATOM	450	H	ASN	193	13.403	78.487	7.234	1.00	0.00	A
5	ATOM	451	CA	ASN	193	12.935	77.071	5.736	1.00	35.22	A
	ATOM	452	CB	ASN	193	11.409	77.105	5.534	1.00	38.44	A
	ATOM	453	CG	ASN	193	10.967	78.108	4.484	1.00	42.52	A
	ATOM	454	OD1	ASN	193	10.607	77.735	3.366	1.00	48.03	A
	ATOM	455	ND2	ASN	193	10.987	79.383	4.840	1.00	45.99	A
10	ATOM	456	HD21	ASN	193	11.275	79.633	5.739	1.00	0.00	A
	ATOM	457	HD22	ASN	193	10.705	80.040	4.172	1.00	0.00	A
	ATOM	458	C	ASN	193	13.674	77.964	4.718	1.00	31.48	A
	ATOM	459	O	ASN	193	14.389	78.885	5.114	1.00	32.85	A
	ATOM	460	N	VAL	194	13.516	77.699	3.423	1.00	28.41	A
15	ATOM	461	H	VAL	194	12.921	76.971	3.148	1.00	0.00	A
	ATOM	462	CA	VAL	194	14.216	78.485	2.408	1.00	30.39	A
	ATOM	463	CB	VAL	194	15.300	77.621	1.682	1.00	35.86	A
	ATOM	464	CG1	VAL	194	16.253	78.517	0.890	1.00	34.87	A
	ATOM	465	CG2	VAL	194	16.086	76.798	2.700	1.00	31.70	A
20	ATOM	466	C	VAL	194	13.312	79.100	1.347	1.00	26.35	A
	ATOM	467	O	VAL	194	12.352	78.487	0.911	1.00	25.27	A
	ATOM	468	N	THR	195	13.629	80.327	0.938	1.00	30.82	A
	ATOM	469	H	THR	195	14.396	80.780	1.344	1.00	0.00	A
	ATOM	470	CA	THR	195	12.861	81.013	-0.097	1.00	32.80	A
25	ATOM	471	CB	THR	195	11.875	82.059	0.520	1.00	32.61	A
	ATOM	472	OG1	THR	195	12.435	83.370	0.439	1.00	36.07	A
	ATOM	473	HG1	THR	195	11.821	84.005	0.819	1.00	0.00	A
	ATOM	474	CG2	THR	195	11.581	81.730	1.969	1.00	35.80	A
	ATOM	475	C	THR	195	13.832	81.698	-1.066	1.00	34.36	A
30	ATOM	476	O	THR	195	14.830	82.274	-0.638	1.00	37.20	A
	ATOM	477	N	HIS	196	13.562	81.610	-2.368	1.00	31.83	A
	ATOM	478	H	HIS	196	12.767	81.117	-2.664	1.00	0.00	A
	ATOM	479	CA	HIS	196	14.430	82.235	-3.364	1.00	33.42	A
	ATOM	480	CB	HIS	196	14.373	81.488	-4.703	1.00	36.34	A
35	ATOM	481	CG	HIS	196	14.682	80.027	-4.612	1.00	32.56	A
	ATOM	482	CD2	HIS	196	13.920	78.975	-4.231	1.00	33.30	A
	ATOM	483	ND1	HIS	196	15.885	79.493	-5.025	1.00	30.72	A
	ATOM	484	HD1	HIS	196	16.646	80.005	-5.357	1.00	0.00	A
	ATOM	485	CE1	HIS	196	15.850	78.181	-4.905	1.00	27.16	A
40	ATOM	486	NE2	HIS	196	14.669	77.839	-4.425	1.00	24.32	A
	ATOM	487	HE2	HIS	196	14.366	76.932	-4.234	1.00	0.00	A
	ATOM	488	C	HIS	196	13.990	83.676	-3.600	1.00	33.69	A
	ATOM	489	O	HIS	196	12.907	83.910	-4.147	1.00	30.28	A
	ATOM	490	N	GLU	197	14.825	84.633	-3.193	1.00	32.40	A
45	ATOM	491	H	GLU	197	15.670	84.376	-2.769	1.00	0.00	A
	ATOM	492	CA	GLU	197	14.522	86.053	-3.357	1.00	28.21	A
	ATOM	493	CB	GLU	197	15.485	86.884	-2.515	1.00	30.79	A
	ATOM	494	CG	GLU	197	15.369	86.601	-1.025	1.00	29.25	A
	ATOM	495	CD	GLU	197	13.980	86.880	-0.489	1.00	28.81	A
50	ATOM	496	OE1	GLU	197	13.154	87.429	-1.246	1.00	27.20	A
	ATOM	497	OE2	GLU	197	13.712	86.550	0.688	1.00	31.09	A
	ATOM	498	C	GLU	197	14.578	86.469	-4.831	1.00	25.47	A
	ATOM	499	O	GLU	197	13.872	87.380	-5.250	1.00	33.41	A
	ATOM	500	N	PHE	198	15.447	85.817	-5.594	1.00	28.05	A
55	ATOM	501	H	PHE	198	16.035	85.161	-5.166	1.00	0.00	A
	ATOM	502	CA	PHE	198	15.573	86.023	-7.038	1.00	29.94	A
	ATOM	503	CB	PHE	198	15.668	87.522	-7.420	1.00	22.28	A
	ATOM	504	CG	PHE	198	16.939	88.213	-7.021	1.00	20.44	A
	ATOM	505	CD1	PHE	198	18.134	87.969	-7.696	1.00	29.59	A
60	ATOM	506	CD2	PHE	198	16.925	89.166	-6.015	1.00	12.83	A
	ATOM	507	CE1	PHE	198	19.300	88.669	-7.376	1.00	23.18	A
	ATOM	508	CE2	PHE	198	18.074	89.872	-5.683	1.00	23.57	A
	ATOM	509	CZ	PHE	198	19.269	89.626	-6.364	1.00	26.69	A
	ATOM	510	C	PHE	198	16.684	85.181	-7.679	1.00	34.58	A
65	ATOM	511	O	PHE	198	17.787	85.048	-7.131	1.00	35.32	A
	ATOM	512	N	ASN	199	16.352	84.590	-8.828	1.00	33.63	A
	ATOM	513	H	ASN	199	15.456	84.756	-9.187	1.00	0.00	A
	ATOM	514	CA	ASN	199	17.237	83.708	-9.592	1.00	33.60	A
	ATOM	515	CB	ASN	199	16.416	82.890	-10.596	1.00	33.43	A
70	ATOM	516	CG	ASN	199	15.406	81.979	-9.929	1.00	35.08	A
	ATOM	517	OD1	ASN	199	15.458	81.743	-8.724	1.00	37.14	A
	ATOM	518	ND2	ASN	199	14.480	81.457	-10.717	1.00	36.96	A
	ATOM	519	HD21	ASN	199	14.477	81.669	-11.674	1.00	0.00	A

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	ATOM	520	HD22	ASN	199	13.818	80.865	-10.306	1.00	0.00	A
	ATOM	521	C	ASN	199	18.381	84.392	-10.352	1.00	37.18	A
	ATOM	522	O	ASN	199	18.312	85.573	-10.690	1.00	33.75	A
5	ATOM	523	N	LEU	200	19.413	83.605	-10.649	1.00	35.28	A
	ATOM	524	H	LEU	200	19.374	82.663	-10.382	1.00	0.00	A
	ATOM	525	CA	LEU	200	20.595	84.080	-11.357	1.00	36.97	A
	ATOM	526	CB	LEU	200	21.612	82.943	-11.502	1.00	36.01	A
	ATOM	527	CG	LEU	200	22.358	82.306	-10.328	1.00	32.50	A
10	ATOM	528	CD1	LEU	200	21.430	81.966	-9.168	1.00	38.36	A
	ATOM	529	CD2	LEU	200	22.997	81.034	-10.851	1.00	33.04	A
	ATOM	530	C	LEU	200	20.304	84.640	-12.746	1.00	36.89	A
	ATOM	531	O	LEU	200	21.069	85.453	-13.256	1.00	38.59	A
	ATOM	532	N	ASN	201	19.217	84.196	-13.370	1.00	38.74	A
15	ATOM	533	H	ASN	201	18.633	83.546	-12.929	1.00	0.00	A
	ATOM	534	CA	ASN	201	18.891	84.676	-14.713	1.00	40.95	A
	ATOM	535	CB	ASN	201	18.643	83.497	-15.666	1.00	42.74	A
	ATOM	536	CG	ASN	201	17.424	82.664	-15.284	1.00	45.08	A
	ATOM	537	OD1	ASN	201	17.100	81.693	-15.969	1.00	46.68	A
20	ATOM	538	ND2	ASN	201	16.746	83.032	-14.199	1.00	42.33	A
	ATOM	539	HD21	ASN	201	17.038	83.811	-13.682	1.00	0.00	A
	ATOM	540	HD22	ASN	201	15.963	82.499	-13.952	1.00	0.00	A
	ATOM	541	C	ASN	201	17.696	85.616	-14.726	1.00	41.99	A
	ATOM	542	O	ASN	201	17.194	85.997	-15.785	1.00	36.95	A
25	ATOM	543	N	LYS	202	17.257	85.993	-13.532	1.00	43.02	A
	ATOM	544	H	LYS	202	17.711	85.657	-12.731	1.00	0.00	A
	ATOM	545	CA	LYS	202	16.127	86.889	-13.378	1.00	42.25	A
	ATOM	546	CB	LYS	202	15.743	86.957	-11.896	1.00	37.84	A
	ATOM	547	CG	LYS	202	14.984	88.195	-11.505	1.00	39.09	A
30	ATOM	548	CD	LYS	202	13.486	88.011	-11.664	1.00	41.90	A
	ATOM	549	CE	LYS	202	12.851	87.494	-10.381	1.00	47.46	A
	ATOM	550	NZ	LYS	202	12.961	86.005	-10.253	1.00	45.02	A
	ATOM	551	HZ1	LYS	202	13.963	85.729	-10.250	1.00	0.00	A
	ATOM	552	HZ2	LYS	202	12.479	85.552	-11.057	1.00	0.00	A
35	ATOM	553	HZ3	LYS	202	12.513	85.699	-9.366	1.00	0.00	A
	ATOM	554	C	LYS	202	16.443	88.287	-13.921	1.00	40.53	A
	ATOM	555	O	LYS	202	15.698	88.829	-14.735	1.00	36.63	A
	ATOM	556	N	TYR	203	17.558	88.864	-13.486	1.00	41.00	A
	ATOM	557	H	TYR	203	18.140	88.383	-12.861	1.00	0.00	A
40	ATOM	558	CA	TYR	203	17.923	90.201	-13.931	1.00	40.78	A
	ATOM	559	CB	TYR	203	18.101	91.114	-12.711	1.00	43.99	A
	ATOM	560	CG	TYR	203	16.946	91.108	-11.723	1.00	42.62	A
	ATOM	561	CD1	TYR	203	17.064	90.475	-10.483	1.00	42.17	A
	ATOM	562	CE1	TYR	203	16.027	90.492	-9.556	1.00	36.22	A
45	ATOM	563	CD2	TYR	203	15.750	91.761	-12.010	1.00	44.83	A
	ATOM	564	CE2	TYR	203	14.702	91.786	-11.086	1.00	48.25	A
	ATOM	565	CZ	TYR	203	14.848	91.151	-9.860	1.00	47.45	A
	ATOM	566	OH	TYR	203	13.815	91.181	-8.942	1.00	52.58	A
	ATOM	567	HH	TYR	203	13.077	91.678	-9.304	1.00	0.00	A
50	ATOM	568	C	TYR	203	19.181	90.243	-14.813	1.00	42.72	A
	ATOM	569	O	TYR	203	20.014	89.335	-14.784	1.00	38.83	A
	ATOM	570	N	SER	204	19.313	91.312	-15.591	1.00	43.42	A
	ATOM	571	H	SER	204	18.628	92.013	-15.556	1.00	0.00	A
	ATOM	572	CA	SER	204	20.445	91.476	-16.499	1.00	45.46	A
55	ATOM	573	CB	SER	204	19.945	91.613	-17.933	1.00	47.15	A
	ATOM	574	OG	SER	204	19.893	92.982	-18.309	1.00	49.62	A
	ATOM	575	HG	SER	204	20.770	93.366	-18.244	1.00	0.00	A
	ATOM	576	C	SER	204	21.312	92.691	-16.188	1.00	49.08	A
	ATOM	577	O	SER	204	22.464	92.760	-16.616	1.00	48.50	A
60	ATOM	578	N	SER	205	20.757	93.656	-15.462	1.00	50.50	A
	ATOM	579	H	SER	205	19.839	93.549	-15.138	1.00	0.00	A
	ATOM	580	CA	SER	205	21.495	94.870	-15.141	1.00	49.60	A
	ATOM	581	CB	SER	205	20.634	96.098	-15.449	1.00	49.35	A
	ATOM	582	OG	SER	205	21.303	96.970	-16.345	1.00	54.35	A
65	ATOM	583	HG	SER	205	22.128	97.262	-15.950	1.00	0.00	A
	ATOM	584	C	SER	205	21.981	94.944	-13.699	1.00	47.82	A
	ATOM	585	O	SER	205	21.316	94.469	-12.785	1.00	41.96	A
	ATOM	586	N	THR	206	23.151	95.547	-13.512	1.00	46.13	A
	ATOM	587	H	THR	206	23.643	95.889	-14.287	1.00	0.00	A
70	ATOM	588	CA	THR	206	23.715	95.710	-12.184	1.00	49.52	A
	ATOM	589	CB	THR	206	25.121	96.351	-12.233	1.00	46.33	A
	ATOM	590	OG1	THR	206	26.115	95.324	-12.316	1.00	47.49	A
	ATOM	591	HG1	THR	206	26.050	94.753	-11.545	1.00	0.00	A
	ATOM	592	CG2	THR	206	25.381	97.172	-10.980	1.00	46.12	A

1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 11. 12. 13. 14. 15. 16. 17. 18. 19. 20. 21. 22. 23. 24. 25. 26. 27. 28. 29. 30. 31. 32. 33. 34. 35. 36. 37. 38. 39. 40. 41. 42. 43. 44. 45. 46. 47. 48. 49. 50. 51. 52. 53. 54. 55. 56. 57. 58. 59. 60. 61. 62. 63. 64. 65. 66. 67. 68. 69. 70. 71. 72. 73. 74. 75. 76. 77. 78. 79. 80. 81. 82. 83. 84. 85. 86. 87. 88. 89. 90. 91. 92. 93. 94. 95. 96. 97. 98. 99. 100.

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|----|------|-----|------|-----|-----|--------|---------|---------|------|-------|---|
| 5 | ATOM | 593 | C | THR | 206 | 22.792 | 96.617 | -11.383 | 1.00 | 49.12 | A |
| | ATOM | 594 | O | THR | 206 | 22.684 | 96.479 | -10.166 | 1.00 | 53.03 | A |
| | ATOM | 595 | N | GLU | 207 | 22.123 | 97.538 | -12.070 | 1.00 | 51.42 | A |
| | ATOM | 596 | H | GLU | 207 | 22.243 | 97.592 | -13.042 | 1.00 | 0.00 | A |
| | ATOM | 597 | CA | GLU | 207 | 21.215 | 98.469 | -11.408 | 1.00 | 49.16 | A |
| 10 | ATOM | 598 | CB | GLU | 207 | 21.002 | 99.720 | -12.269 | 1.00 | 52.87 | A |
| | ATOM | 599 | CG | GLU | 207 | 21.187 | 99.521 | -13.762 | 1.00 | 55.52 | A |
| | ATOM | 600 | CD | GLU | 207 | 20.886 | 100.782 | -14.550 | 1.00 | 56.44 | A |
| | ATOM | 601 | OE1 | GLU | 207 | 21.844 | 101.489 | -14.932 | 1.00 | 55.48 | A |
| | ATOM | 602 | OE2 | GLU | 207 | 19.692 | 101.066 | -14.784 | 1.00 | 53.55 | A |
| 15 | ATOM | 603 | C | GLU | 207 | 19.864 | 97.858 | -11.066 | 1.00 | 49.23 | A |
| | ATOM | 604 | O | GLU | 207 | 19.350 | 98.053 | -9.964 | 1.00 | 48.23 | A |
| | ATOM | 605 | N | GLU | 208 | 19.276 | 97.122 | -12.000 | 1.00 | 47.83 | A |
| | ATOM | 606 | H | GLU | 208 | 19.710 | 96.988 | -12.870 | 1.00 | 0.00 | A |
| | ATOM | 607 | CA | GLU | 208 | 17.981 | 96.511 | -11.727 | 1.00 | 48.69 | A |
| 20 | ATOM | 608 | CB | GLU | 208 | 17.500 | 95.700 | -12.916 | 1.00 | 45.35 | A |
| | ATOM | 609 | CG | GLU | 208 | 17.020 | 96.510 | -14.082 | 1.00 | 40.10 | A |
| | ATOM | 610 | CD | GLU | 208 | 16.724 | 95.620 | -15.262 | 1.00 | 37.99 | A |
| | ATOM | 611 | OE1 | GLU | 208 | 15.676 | 95.799 | -15.918 | 1.00 | 46.28 | A |
| | ATOM | 612 | OE2 | GLU | 208 | 17.545 | 94.727 | -15.528 | 1.00 | 36.45 | A |
| 25 | ATOM | 613 | C | GLU | 208 | 18.129 | 95.584 | -10.535 | 1.00 | 50.21 | A |
| | ATOM | 614 | O | GLU | 208 | 17.317 | 95.603 | -9.608 | 1.00 | 50.81 | A |
| | ATOM | 615 | N | VAL | 209 | 19.174 | 94.764 | -10.573 | 1.00 | 47.53 | A |
| | ATOM | 616 | H | VAL | 209 | 19.778 | 94.788 | -11.344 | 1.00 | 0.00 | A |
| | ATOM | 617 | CA | VAL | 209 | 19.436 | 93.832 | -9.489 | 1.00 | 48.06 | A |
| 30 | ATOM | 618 | CB | VAL | 209 | 20.744 | 93.024 | -9.738 | 1.00 | 48.35 | A |
| | ATOM | 619 | CG1 | VAL | 209 | 21.363 | 92.582 | -8.421 | 1.00 | 49.78 | A |
| | ATOM | 620 | CG2 | VAL | 209 | 20.446 | 91.809 | -10.589 | 1.00 | 49.88 | A |
| | ATOM | 621 | C | VAL | 209 | 19.549 | 94.619 | -8.187 | 1.00 | 45.25 | A |
| | ATOM | 622 | O | VAL | 209 | 19.145 | 94.138 | -7.134 | 1.00 | 43.45 | A |
| 35 | ATOM | 623 | N | LEU | 210 | 20.081 | 95.836 | -8.263 | 1.00 | 45.57 | A |
| | ATOM | 624 | H | LEU | 210 | 20.373 | 96.189 | -9.130 | 1.00 | 0.00 | A |
| | ATOM | 625 | CA | LEU | 210 | 20.232 | 96.652 | -7.061 | 1.00 | 46.10 | A |
| | ATOM | 626 | CB | LEU | 210 | 21.031 | 97.931 | -7.356 | 1.00 | 44.07 | A |
| | ATOM | 627 | CG | LEU | 210 | 22.557 | 97.828 | -7.549 | 1.00 | 44.26 | A |
| 40 | ATOM | 628 | CD1 | LEU | 210 | 23.131 | 99.226 | -7.738 | 1.00 | 38.37 | A |
| | ATOM | 629 | CD2 | LEU | 210 | 23.218 | 97.138 | -6.361 | 1.00 | 35.26 | A |
| | ATOM | 630 | C | LEU | 210 | 18.862 | 97.006 | -6.490 | 1.00 | 44.20 | A |
| | ATOM | 631 | O | LEU | 210 | 18.653 | 96.925 | -5.286 | 1.00 | 44.77 | A |
| | ATOM | 632 | N | VAL | 211 | 17.928 | 97.389 | -7.349 | 1.00 | 45.51 | A |
| 45 | ATOM | 633 | H | VAL | 211 | 18.137 | 97.445 | -8.305 | 1.00 | 0.00 | A |
| | ATOM | 634 | CA | VAL | 211 | 16.591 | 97.731 | -6.880 | 1.00 | 44.84 | A |
| | ATOM | 635 | CB | VAL | 211 | 15.685 | 98.253 | -8.021 | 1.00 | 44.98 | A |
| | ATOM | 636 | CG1 | VAL | 211 | 14.649 | 99.213 | -7.449 | 1.00 | 49.23 | A |
| | ATOM | 637 | CG2 | VAL | 211 | 16.517 | 98.940 | -9.095 | 1.00 | 47.62 | A |
| 50 | ATOM | 638 | C | VAL | 211 | 15.914 | 96.503 | -6.278 | 1.00 | 42.72 | A |
| | ATOM | 639 | O | VAL | 211 | 15.219 | 96.595 | -5.262 | 1.00 | 42.50 | A |
| | ATOM | 640 | N | ALA | 212 | 16.122 | 95.353 | -6.907 | 1.00 | 40.62 | A |
| | ATOM | 641 | H | ALA | 212 | 16.699 | 95.334 | -7.699 | 1.00 | 0.00 | A |
| | ATOM | 642 | CA | ALA | 212 | 15.509 | 94.116 | -6.440 | 1.00 | 40.77 | A |
| 55 | ATOM | 643 | CB | ALA | 212 | 15.742 | 93.011 | -7.454 | 1.00 | 36.33 | A |
| | ATOM | 644 | C | ALA | 212 | 16.001 | 93.672 | -5.063 | 1.00 | 38.58 | A |
| | ATOM | 645 | O | ALA | 212 | 15.207 | 93.243 | -4.221 | 1.00 | 37.62 | A |
| | ATOM | 646 | N | ALA | 213 | 17.305 | 93.779 | -4.837 | 1.00 | 31.59 | A |
| | ATOM | 647 | H | ALA | 213 | 17.889 | 94.145 | -5.532 | 1.00 | 0.00 | A |
| 60 | ATOM | 648 | CA | ALA | 213 | 17.879 | 93.359 | -3.564 | 1.00 | 35.24 | A |
| | ATOM | 649 | CB | ALA | 213 | 19.386 | 93.229 | -3.687 | 1.00 | 35.74 | A |
| | ATOM | 650 | C | ALA | 213 | 17.540 | 94.277 | -2.404 | 1.00 | 33.73 | A |
| | ATOM | 651 | O | ALA | 213 | 17.515 | 93.837 | -1.264 | 1.00 | 30.39 | A |
| | ATOM | 652 | N | ASN | 214 | 17.277 | 95.548 | -2.688 | 1.00 | 37.82 | A |
| 65 | ATOM | 653 | H | ASN | 214 | 17.292 | 95.854 | -3.618 | 1.00 | 0.00 | A |
| | ATOM | 654 | CA | ASN | 214 | 16.962 | 96.495 | -1.620 | 1.00 | 41.93 | A |
| | ATOM | 655 | CB | ASN | 214 | 17.152 | 97.935 | -2.102 | 1.00 | 43.82 | A |
| | ATOM | 656 | CG | ASN | 214 | 18.495 | 98.509 | -1.688 | 1.00 | 45.59 | A |
| | ATOM | 657 | OD1 | ASN | 214 | 19.426 | 98.581 | -2.492 | 1.00 | 47.44 | A |
| 70 | ATOM | 658 | ND2 | ASN | 214 | 18.606 | 98.911 | -0.425 | 1.00 | 46.09 | A |
| | ATOM | 659 | HD21 | ASN | 214 | 17.842 | 98.829 | 0.183 | 1.00 | 0.00 | A |
| | ATOM | 660 | HD22 | ASN | 214 | 19.465 | 99.284 | -0.143 | 1.00 | 0.00 | A |
| | ATOM | 661 | C | ASN | 214 | 15.555 | 96.313 | -1.084 | 1.00 | 44.23 | A |
| | ATOM | 662 | O | ASN | 214 | 15.232 | 96.808 | -0.009 | 1.00 | 45.11 | A |
| | ATOM | 663 | N | LYS | 215 | 14.724 | 95.589 | -1.830 | 1.00 | 44.69 | A |
| | ATOM | 664 | H | LYS | 215 | 15.045 | 95.212 | -2.677 | 1.00 | 0.00 | A |
| | ATOM | 665 | CA | LYS | 215 | 13.351 | 95.347 | -1.416 | 1.00 | 43.68 | A |

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|----|------|-----|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 666 | CB | LYS | 215 | 12.425 | 95.401 | -2.632 | 1.00 | 45.74 | A |
| | ATOM | 667 | CG | LYS | 215 | 12.506 | 94.172 | -3.524 | 1.00 | 54.82 | A |
| | ATOM | 668 | CD | LYS | 215 | 12.162 | 94.511 | -4.971 | 1.00 | 55.87 | A |
| | ATOM | 669 | CE | LYS | 215 | 11.845 | 93.258 | -5.776 | 1.00 | 59.40 | A |
| | ATOM | 670 | NZ | LYS | 215 | 10.388 | 92.928 | -5.762 | 1.00 | 58.33 | A |
| 10 | ATOM | 671 | HZ1 | LYS | 215 | 9.850 | 93.718 | -6.173 | 1.00 | 0.00 | A |
| | ATOM | 672 | HZ2 | LYS | 215 | 10.077 | 92.768 | -4.784 | 1.00 | 0.00 | A |
| | ATOM | 673 | HZ3 | LYS | 215 | 10.223 | 92.068 | -6.323 | 1.00 | 0.00 | A |
| | ATOM | 674 | C | LYS | 215 | 13.184 | 94.007 | -0.701 | 1.00 | 41.09 | A |
| | ATOM | 675 | O | LYS | 215 | 12.073 | 93.505 | -0.575 | 1.00 | 41.46 | A |
| 15 | ATOM | 676 | N | ILE | 216 | 14.280 | 93.427 | -0.227 | 1.00 | 38.99 | A |
| | ATOM | 677 | H | ILE | 216 | 15.151 | 93.863 | -0.342 | 1.00 | 0.00 | A |
| | ATOM | 678 | CA | ILE | 216 | 14.197 | 92.146 | 0.463 | 1.00 | 34.14 | A |
| | ATOM | 679 | CB | ILE | 216 | 15.477 | 91.305 | 0.281 | 1.00 | 34.52 | A |
| | ATOM | 680 | CG2 | ILE | 216 | 15.367 | 90.029 | 1.102 | 1.00 | 30.52 | A |
| 20 | ATOM | 681 | CG1 | ILE | 216 | 15.694 | 90.973 | -1.192 | 1.00 | 29.14 | A |
| | ATOM | 682 | CD1 | ILE | 216 | 17.084 | 90.443 | -1.481 | 1.00 | 27.72 | A |
| | ATOM | 683 | C | ILE | 216 | 13.987 | 92.335 | 1.952 | 1.00 | 31.56 | A |
| | ATOM | 684 | O | ILE | 216 | 14.823 | 92.918 | 2.637 | 1.00 | 31.71 | A |
| | ATOM | 685 | N | GLY | 217 | 12.874 | 91.824 | 2.458 | 1.00 | 33.70 | A |
| 25 | ATOM | 686 | H | GLY | 217 | 12.242 | 91.354 | 1.875 | 1.00 | 0.00 | A |
| | ATOM | 687 | CA | GLY | 217 | 12.595 | 91.962 | 3.872 | 1.00 | 36.08 | A |
| | ATOM | 688 | C | GLY | 217 | 13.014 | 90.749 | 4.680 | 1.00 | 38.70 | A |
| | ATOM | 689 | O | GLY | 217 | 13.112 | 89.642 | 4.141 | 1.00 | 38.11 | A |
| | ATOM | 690 | N | ARG | 218 | 13.269 | 90.965 | 5.968 | 1.00 | 37.58 | A |
| 30 | ATOM | 691 | H | ARG | 218 | 13.193 | 91.876 | 6.318 | 1.00 | 0.00 | A |
| | ATOM | 692 | CA | ARG | 218 | 13.667 | 89.895 | 6.884 | 1.00 | 38.94 | A |
| | ATOM | 693 | CB | ARG | 218 | 13.990 | 90.473 | 8.267 | 1.00 | 37.57 | A |
| | ATOM | 694 | CG | ARG | 218 | 14.512 | 89.462 | 9.295 | 1.00 | 40.84 | A |
| | ATOM | 695 | CD | ARG | 218 | 15.880 | 89.885 | 9.830 | 1.00 | 43.84 | A |
| 35 | ATOM | 696 | NE | ARG | 218 | 16.011 | 89.820 | 11.283 | 1.00 | 35.18 | A |
| | ATOM | 697 | HE | ARG | 218 | 16.023 | 88.935 | 11.701 | 1.00 | 0.00 | A |
| | ATOM | 698 | CZ | ARG | 218 | 16.126 | 90.882 | 12.073 | 1.00 | 36.87 | A |
| | ATOM | 699 | NH1 | ARG | 218 | 16.126 | 92.114 | 11.573 | 1.00 | 27.19 | A |
| | ATOM | 700 | HH11 | ARG | 218 | 16.055 | 92.253 | 10.583 | 1.00 | 0.00 | A |
| 40 | ATOM | 701 | HH12 | ARG | 218 | 16.212 | 92.903 | 12.181 | 1.00 | 0.00 | A |
| | ATOM | 702 | NH2 | ARG | 218 | 16.263 | 90.706 | 13.374 | 1.00 | 41.63 | A |
| | ATOM | 703 | HH21 | ARG | 218 | 16.287 | 89.785 | 13.753 | 1.00 | 0.00 | A |
| | ATOM | 704 | HH22 | ARG | 218 | 16.345 | 91.499 | 13.979 | 1.00 | 0.00 | A |
| | ATOM | 705 | C | ARG | 218 | 12.546 | 88.873 | 7.006 | 1.00 | 35.63 | A |
| 45 | ATOM | 706 | O | ARG | 218 | 11.488 | 89.167 | 7.556 | 1.00 | 43.27 | A |
| | ATOM | 707 | N | GLN | 219 | 12.788 | 87.667 | 6.504 | 1.00 | 39.56 | A |
| | ATOM | 708 | H | GLN | 219 | 13.661 | 87.489 | 6.097 | 1.00 | 0.00 | A |
| | ATOM | 709 | CA | GLN | 219 | 11.792 | 86.602 | 6.541 | 1.00 | 38.70 | A |
| | ATOM | 710 | CB | GLN | 219 | 12.265 | 85.411 | 5.694 | 1.00 | 33.61 | A |
| 50 | ATOM | 711 | CG | GLN | 219 | 12.960 | 84.295 | 6.452 | 1.00 | 32.85 | A |
| | ATOM | 712 | CD | GLN | 219 | 12.950 | 82.995 | 5.682 | 1.00 | 33.39 | A |
| | ATOM | 713 | OE1 | GLN | 219 | 12.946 | 82.990 | 4.449 | 1.00 | 38.03 | A |
| | ATOM | 714 | NE2 | GLN | 219 | 12.938 | 81.883 | 6.402 | 1.00 | 39.97 | A |
| | ATOM | 715 | HE21 | GLN | 219 | 12.936 | 81.933 | 7.380 | 1.00 | 0.00 | A |
| 55 | ATOM | 716 | HE22 | GLN | 219 | 12.931 | 81.032 | 5.917 | 1.00 | 0.00 | A |
| | ATOM | 717 | C | GLN | 219 | 11.465 | 86.161 | 7.961 | 1.00 | 41.40 | A |
| | ATOM | 718 | O | GLN | 219 | 10.317 | 85.831 | 8.269 | 1.00 | 40.86 | A |
| | ATOM | 719 | N | GLY | 220 | 12.470 | 86.161 | 8.828 | 1.00 | 40.86 | A |
| | ATOM | 720 | H | GLY | 220 | 13.369 | 86.424 | 8.536 | 1.00 | 0.00 | A |
| 60 | ATOM | 721 | CA | GLY | 220 | 12.241 | 85.771 | 10.206 | 1.00 | 40.81 | A |
| | ATOM | 722 | C | GLY | 220 | 12.464 | 84.299 | 10.470 | 1.00 | 41.52 | A |
| | ATOM | 723 | O | GLY | 220 | 12.137 | 83.447 | 9.650 | 1.00 | 37.96 | A |
| | ATOM | 724 | N | GLY | 221 | 13.022 | 84.001 | 11.634 | 1.00 | 44.63 | A |
| | ATOM | 725 | H | GLY | 221 | 13.258 | 84.716 | 12.260 | 1.00 | 0.00 | A |
| 65 | ATOM | 726 | CA | GLY | 221 | 13.282 | 82.623 | 11.987 | 1.00 | 43.63 | A |
| | ATOM | 727 | C | GLY | 221 | 13.912 | 82.468 | 13.354 | 1.00 | 44.55 | A |
| | ATOM | 728 | O | GLY | 221 | 14.805 | 83.221 | 13.742 | 1.00 | 40.07 | A |
| | ATOM | 729 | N | LEU | 222 | 13.416 | 81.477 | 14.085 | 1.00 | 45.22 | A |
| | ATOM | 730 | H | LEU | 222 | 12.691 | 80.940 | 13.711 | 1.00 | 0.00 | A |
| 70 | ATOM | 731 | CA | LEU | 222 | 13.903 | 81.151 | 15.411 | 1.00 | 47.35 | A |
| | ATOM | 732 | CB | LEU | 222 | 12.781 | 80.471 | 16.207 | 1.00 | 54.79 | A |
| | ATOM | 733 | CG | LEU | 222 | 11.395 | 80.687 | 15.579 | 0.01 | 54.77 | A |
| | ATOM | 734 | CD1 | LEU | 222 | 10.343 | 79.881 | 16.311 | 0.01 | 55.93 | A |
| | ATOM | 735 | CD2 | LEU | 222 | 11.048 | 82.171 | 15.608 | 0.01 | 57.10 | A |
| | ATOM | 736 | C | LEU | 222 | 15.066 | 80.194 | 15.172 | 1.00 | 47.02 | A |
| | ATOM | 737 | O | LEU | 222 | 16.135 | 80.340 | 15.757 | 1.00 | 47.47 | A |
| | ATOM | 738 | N | GLN | 223 | 14.837 | 79.233 | 14.279 | 1.00 | 42.82 | A |

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|----|------|-----|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 739 | H | GLN | 223 | 13.955 | 79.189 | 13.857 | 1.00 | 0.00 | A |
| | ATOM | 740 | CA | GLN | 223 | 15.837 | 78.241 | 13.903 | 1.00 | 40.39 | A |
| | ATOM | 741 | CB | GLN | 223 | 15.159 | 76.915 | 13.533 | 1.00 | 38.83 | A |
| | ATOM | 742 | CG | GLN | 223 | 14.256 | 76.346 | 14.617 | 0.01 | 40.23 | A |
| | ATOM | 743 | CD | GLN | 223 | 13.344 | 75.250 | 14.099 | 0.01 | 40.15 | A |
| 10 | ATOM | 744 | OE1 | GLN | 223 | 13.163 | 74.219 | 14.747 | 0.01 | 39.83 | A |
| | ATOM | 745 | NE2 | GLN | 223 | 12.765 | 75.470 | 12.924 | 0.01 | 39.93 | A |
| | ATOM | 746 | HE21 | GLN | 223 | 12.935 | 76.302 | 12.443 | 1.00 | 0.00 | A |
| | ATOM | 747 | HE22 | GLN | 223 | 12.171 | 74.771 | 12.577 | 1.00 | 0.00 | A |
| | ATOM | 748 | C | GLN | 223 | 16.666 | 78.746 | 12.713 | 1.00 | 40.39 | A |
| 15 | ATOM | 749 | O | GLN | 223 | 16.144 | 79.404 | 11.804 | 1.00 | 38.90 | A |
| | ATOM | 750 | N | THR | 224 | 17.954 | 78.413 | 12.722 | 1.00 | 32.13 | A |
| | ATOM | 751 | H | THR | 224 | 18.293 | 77.864 | 13.458 | 1.00 | 0.00 | A |
| | ATOM | 752 | CA | THR | 224 | 18.885 | 78.836 | 11.675 | 1.00 | 29.74 | A |
| | ATOM | 753 | CB | THR | 224 | 20.006 | 79.688 | 12.333 | 1.00 | 28.84 | A |
| 20 | ATOM | 754 | OG1 | THR | 224 | 19.462 | 80.968 | 12.668 | 1.00 | 31.13 | A |
| | ATOM | 755 | HG1 | THR | 224 | 19.146 | 81.401 | 11.872 | 1.00 | 0.00 | A |
| | ATOM | 756 | CG2 | THR | 224 | 21.205 | 79.867 | 11.415 | 1.00 | 24.03 | A |
| | ATOM | 757 | C | THR | 224 | 19.450 | 77.608 | 10.940 | 1.00 | 25.16 | A |
| | ATOM | 758 | O | THR | 224 | 20.438 | 77.013 | 11.366 | 1.00 | 21.68 | A |
| 25 | ATOM | 759 | N | MET | 225 | 18.809 | 77.231 | 9.837 | 1.00 | 23.33 | A |
| | ATOM | 760 | H | MET | 225 | 18.044 | 77.757 | 9.525 | 1.00 | 0.00 | A |
| | ATOM | 761 | CA | MET | 225 | 19.219 | 76.051 | 9.082 | 1.00 | 25.92 | A |
| | ATOM | 762 | CB | MET | 225 | 17.979 | 75.377 | 8.504 | 1.00 | 26.36 | A |
| | ATOM | 763 | CG | MET | 225 | 16.851 | 75.275 | 9.495 | 1.00 | 24.17 | A |
| 30 | ATOM | 764 | SD | MET | 225 | 17.187 | 73.904 | 10.572 | 1.00 | 33.11 | A |
| | ATOM | 765 | CE | MET | 225 | 16.928 | 72.552 | 9.456 | 1.00 | 31.18 | A |
| | ATOM | 766 | C | MET | 225 | 20.205 | 76.326 | 7.958 | 1.00 | 26.44 | A |
| | ATOM | 767 | O | MET | 225 | 19.850 | 76.238 | 6.785 | 1.00 | 27.44 | A |
| | ATOM | 768 | N | THR | 226 | 21.446 | 76.640 | 8.303 | 1.00 | 27.96 | A |
| 35 | ATOM | 769 | H | THR | 226 | 21.699 | 76.679 | 9.248 | 1.00 | 0.00 | A |
| | ATOM | 770 | CA | THR | 226 | 22.433 | 76.930 | 7.268 | 1.00 | 26.56 | A |
| | ATOM | 771 | CB | THR | 226 | 23.761 | 77.426 | 7.879 | 1.00 | 28.59 | A |
| | ATOM | 772 | OG1 | THR | 226 | 23.478 | 78.382 | 8.904 | 1.00 | 29.78 | A |
| | ATOM | 773 | HG1 | THR | 226 | 24.301 | 78.693 | 9.288 | 1.00 | 0.00 | A |
| 40 | ATOM | 774 | CG2 | THR | 226 | 24.622 | 78.102 | 6.807 | 1.00 | 25.78 | A |
| | ATOM | 775 | C | THR | 226 | 22.709 | 75.740 | 6.347 | 1.00 | 24.98 | A |
| | ATOM | 776 | O | THR | 226 | 22.912 | 75.922 | 5.152 | 1.00 | 20.19 | A |
| | ATOM | 777 | N | ALA | 227 | 22.709 | 74.525 | 6.889 | 1.00 | 25.81 | A |
| | ATOM | 778 | H | ALA | 227 | 22.547 | 74.412 | 7.848 | 1.00 | 0.00 | A |
| 45 | ATOM | 779 | CA | ALA | 227 | 22.953 | 73.357 | 6.047 | 1.00 | 23.49 | A |
| | ATOM | 780 | CB | ALA | 227 | 22.972 | 72.077 | 6.876 | 1.00 | 23.86 | A |
| | ATOM | 781 | C | ALA | 227 | 21 | | | | | |

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|----|------|-----|-----|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 812 | OD2 | ASP | 231 | 21.722 | 69.124 | 1.183 | 1.00 | 32.43 | A |
| | ATOM | 813 | C | ASP | 231 | 21.149 | 72.943 | -0.900 | 1.00 | 25.92 | A |
| | ATOM | 814 | O | ASP | 231 | 21.167 | 72.412 | -2.019 | 1.00 | 22.17 | A |
| | ATOM | 815 | N | THR | 232 | 20.216 | 73.803 | -0.513 | 1.00 | 30.41 | A |
| | ATOM | 816 | H | THR | 232 | 20.257 | 74.169 | 0.395 | 1.00 | 0.00 | A |
| 10 | ATOM | 817 | CA | THR | 232 | 19.138 | 74.216 | -1.391 | 1.00 | 27.31 | A |
| | ATOM | 818 | CB | THR | 232 | 18.059 | 74.977 | -0.578 | 1.00 | 31.03 | A |
| | ATOM | 819 | OG1 | THR | 232 | 17.404 | 74.051 | 0.299 | 1.00 | 30.78 | A |
| | ATOM | 820 | HG1 | THR | 232 | 16.732 | 74.513 | 0.807 | 1.00 | 0.00 | A |
| | ATOM | 821 | CG2 | THR | 232 | 17.023 | 75.618 | -1.497 | 1.00 | 22.38 | A |
| 15 | ATOM | 822 | C | THR | 232 | 19.716 | 75.095 | -2.502 | 1.00 | 27.81 | A |
| | ATOM | 823 | O | THR | 232 | 19.325 | 74.978 | -3.659 | 1.00 | 27.44 | A |
| | ATOM | 824 | N | ALA | 233 | 20.676 | 75.946 | -2.148 | 1.00 | 27.86 | A |
| | ATOM | 825 | H | ALA | 233 | 20.957 | 75.979 | -1.210 | 1.00 | 0.00 | A |
| | ATOM | 826 | CA | ALA | 233 | 21.321 | 76.830 | -3.112 | 1.00 | 31.80 | A |
| 20 | ATOM | 827 | CB | ALA | 233 | 22.162 | 77.876 | -2.381 | 1.00 | 27.63 | A |
| | ATOM | 828 | C | ALA | 233 | 22.195 | 76.042 | -4.095 | 1.00 | 35.25 | A |
| | ATOM | 829 | O | ALA | 233 | 22.341 | 76.431 | -5.255 | 1.00 | 37.14 | A |
| | ATOM | 830 | N | ALA | 234 | 22.776 | 74.940 | -3.632 | 1.00 | 35.16 | A |
| | ATOM | 831 | H | ALA | 234 | 22.638 | 74.681 | -2.696 | 1.00 | 0.00 | A |
| 25 | ATOM | 832 | CA | ALA | 234 | 23.613 | 74.111 | -4.486 | 1.00 | 37.73 | A |
| | ATOM | 833 | CB | ALA | 234 | 24.552 | 73.271 | -3.651 | 1.00 | 41.51 | A |
| | ATOM | 834 | C | ALA | 234 | 22.712 | 73.205 | -5.293 | 1.00 | 40.15 | A |
| | ATOM | 835 | O | ALA | 234 | 23.045 | 72.806 | -6.407 | 1.00 | 40.08 | A |
| | ATOM | 836 | N | LYS | 235 | 21.556 | 72.897 | -4.719 | 1.00 | 38.44 | A |
| 30 | ATOM | 837 | H | LYS | 235 | 21.342 | 73.275 | -3.841 | 1.00 | 0.00 | A |
| | ATOM | 838 | CA | LYS | 235 | 20.601 | 72.013 | -5.361 | 1.00 | 37.80 | A |
| | ATOM | 839 | CB | LYS | 235 | 19.826 | 71.223 | -4.299 | 1.00 | 39.04 | A |
| | ATOM | 840 | CG | LYS | 235 | 20.401 | 69.856 | -3.977 | 1.00 | 40.19 | A |
| | ATOM | 841 | CD | LYS | 235 | 19.542 | 69.129 | -2.957 | 1.00 | 40.24 | A |
| 35 | ATOM | 842 | CE | LYS | 235 | 19.458 | 67.642 | -3.268 | 1.00 | 40.62 | A |
| | ATOM | 843 | NZ | LYS | 235 | 18.951 | 66.862 | -2.102 | 1.00 | 39.60 | A |
| | ATOM | 844 | HZ1 | LYS | 235 | 17.999 | 67.200 | -1.848 | 1.00 | 0.00 | A |
| | ATOM | 845 | HZ2 | LYS | 235 | 19.591 | 66.994 | -1.293 | 1.00 | 0.00 | A |
| | ATOM | 846 | HZ3 | LYS | 235 | 18.907 | 65.855 | -2.351 | 1.00 | 0.00 | A |
| 40 | ATOM | 847 | C | LYS | 235 | 19.605 | 72.732 | -6.253 | 1.00 | 37.03 | A |
| | ATOM | 848 | O | LYS | 235 | 19.199 | 72.193 | -7.282 | 1.00 | 37.66 | A |
| | ATOM | 849 | N | GLU | 236 | 19.217 | 73.947 | -5.873 | 1.00 | 36.11 | A |
| | ATOM | 850 | H | GLU | 236 | 19.615 | 74.355 | -5.080 | 1.00 | 0.00 | A |
| | ATOM | 851 | CA | GLU | 236 | 18.210 | 74.677 | -6.640 | 1.00 | 39.41 | A |
| 45 | ATOM | 852 | CB | GLU | 236 | 17.025 | 75.022 | -5.736 | 1.00 | 40.91 | A |
| | ATOM | 853 | CG | GLU | 236 | 16.053 | 73.874 | -5.542 | 1.00 | 47.24 | A |
| | ATOM | 854 | CD | GLU | 236 | 15.185 | 74.050 | - | | | |

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|----|------|-----|------|-----|-----|--------|--------|---------|------|-------|---|
| | ATOM | 885 | O | THR | 239 | 19.735 | 76.951 | -13.185 | 1.00 | 46.02 | A |
| | ATOM | 886 | N | GLU | 240 | 20.320 | 75.152 | -14.396 | 1.00 | 48.01 | A |
| | ATOM | 887 | H | GLU | 240 | 20.614 | 74.216 | -14.386 | 1.00 | 0.00 | A |
| | ATOM | 888 | CA | GLU | 240 | 20.123 | 75.825 | -15.667 | 1.00 | 47.10 | A |
| 5 | ATOM | 889 | CB | GLU | 240 | 20.289 | 74.833 | -16.813 | 1.00 | 49.28 | A |
| | ATOM | 890 | CG | GLU | 240 | 21.543 | 73.981 | -16.702 | 1.00 | 56.94 | A |
| | ATOM | 891 | CD | GLU | 240 | 22.735 | 74.606 | -17.398 | 1.00 | 60.51 | A |
| | ATOM | 892 | OE1 | GLU | 240 | 23.662 | 75.079 | -16.700 | 1.00 | 61.18 | A |
| | ATOM | 893 | OE2 | GLU | 240 | 22.741 | 74.625 | -18.645 | 1.00 | 63.05 | A |
| 10 | ATOM | 894 | C | GLU | 240 | 18.737 | 76.427 | -15.691 | 1.00 | 48.10 | A |
| | ATOM | 895 | O | GLU | 240 | 18.482 | 77.397 | -16.397 | 1.00 | 49.86 | A |
| | ATOM | 896 | N | ALA | 241 | 17.848 | 75.844 | -14.893 | 1.00 | 50.22 | A |
| | ATOM | 897 | H | ALA | 241 | 18.132 | 75.082 | -14.346 | 1.00 | 0.00 | A |
| | ATOM | 898 | CA | ALA | 241 | 16.468 | 76.299 | -14.808 | 1.00 | 51.00 | A |
| 15 | ATOM | 899 | CB | ALA | 241 | 15.611 | 75.237 | -14.132 | 1.00 | 48.14 | A |
| | ATOM | 900 | C | ALA | 241 | 16.376 | 77.600 | -14.036 | 1.00 | 49.38 | A |
| | ATOM | 901 | O | ALA | 241 | 15.542 | 78.453 | -14.336 | 1.00 | 52.67 | A |
| | ATOM | 902 | N | ARG | 242 | 17.238 | 77.748 | -13.039 | 1.00 | 43.01 | A |
| | ATOM | 903 | H | ARG | 242 | 17.889 | 77.041 | -12.853 | 1.00 | 0.00 | A |
| 20 | ATOM | 904 | CA | ARG | 242 | 17.226 | 78.944 | -12.221 | 1.00 | 40.74 | A |
| | ATOM | 905 | CB | ARG | 242 | 17.408 | 78.562 | -10.744 | 1.00 | 34.79 | A |
| | ATOM | 906 | CG | ARG | 242 | 16.493 | 77.376 | -10.317 | 1.00 | 30.30 | A |
| | ATOM | 907 | CD | ARG | 242 | 15.817 | 77.532 | -8.931 | 1.00 | 29.76 | A |
| | ATOM | 908 | NE | ARG | 242 | 14.782 | 78.570 | -8.877 | 1.00 | 33.22 | A |
| 25 | ATOM | 909 | HE | ARG | 242 | 14.958 | 79.399 | -9.365 | 1.00 | 0.00 | A |
| | ATOM | 910 | CZ | ARG | 242 | 13.635 | 78.491 | -8.196 | 1.00 | 29.10 | A |
| | ATOM | 911 | NH1 | ARG | 242 | 13.313 | 77.413 | -7.488 | 1.00 | 28.44 | A |
| | ATOM | 912 | HH11 | ARG | 242 | 13.952 | 76.653 | -7.416 | 1.00 | 0.00 | A |
| | ATOM | 913 | HH12 | ARG | 242 | 12.442 | 77.383 | -6.994 | 1.00 | 0.00 | A |
| 30 | ATOM | 914 | NH2 | ARG | 242 | 12.807 | 79.524 | -8.203 | 1.00 | 34.29 | A |
| | ATOM | 915 | HH21 | ARG | 242 | 13.057 | 80.361 | -8.690 | 1.00 | 0.00 | A |
| | ATOM | 916 | HH22 | ARG | 242 | 11.938 | 79.475 | -7.709 | 1.00 | 0.00 | A |
| | ATOM | 917 | C | ARG | 242 | 18.277 | 79.944 | -12.681 | 1.00 | 46.22 | A |
| | ATOM | 918 | O | ARG | 242 | 18.564 | 80.913 | -11.984 | 1.00 | 51.48 | A |
| 35 | ATOM | 919 | N | GLY | 243 | 18.850 | 79.704 | -13.860 | 1.00 | 48.36 | A |
| | ATOM | 920 | H | GLY | 243 | 18.612 | 78.899 | -14.365 | 1.00 | 0.00 | A |
| | ATOM | 921 | CA | GLY | 243 | 19.832 | 80.634 | -14.398 | 1.00 | 45.39 | A |
| | ATOM | 922 | C | GLY | 243 | 21.289 | 80.231 | -14.535 | 1.00 | 43.38 | A |
| | ATOM | 923 | O | GLY | 243 | 21.993 | 80.797 | -15.371 | 1.00 | 43.70 | A |
| 40 | ATOM | 924 | N | ALA | 244 | 21.750 | 79.276 | -13.731 | 1.00 | 41.17 | A |
| | ATOM | 925 | H | ALA | 244 | 21.143 | 78.857 | -13.086 | 1.00 | 0.00 | A |
| | ATOM | 926 | CA | ALA | 244 | 23.144 | 78.838 | -13.789 | 1.00 | 37.01 | A |
| | ATOM | 927 | CB | ALA | 244 | 23.315 | 77.543 | -13.015 | 1.00 | 33.03 | A |
| | ATOM | 928 | C | ALA | 244 | 23.635 | 78.656 | -15.223 | 1.00 | 39.91 | A |
| 45 | ATOM | 929 | O | ALA | 244 | 22.941 | 78.070 | -16.054 | 1.00 | 37.74 | A |
| | ATOM | 930 | N | ARG | 245 | 24.833 | 79.159 | -15.505 | 1.00 | 35.79 | A |
| | ATOM | 931 | H | ARG | 245 | 25.344 | 79.603 | -14.803 | 1.00 | 0.00 | A |
| | ATOM | 932 | CA | ARG | 245 | 25.406 | 79.057 | -16.839 | 1.00 | 37.22 | A |
| | ATOM | 933 | CB | ARG | 245 | 26.112 | 80.375 | -17.205 | 1.00 | 37.87 | A |
| 50 | ATOM | 934 | CG | ARG | 245 | 25.170 | 81.597 | -17.186 | 1.00 | 41.05 | A |
| | ATOM | 935 | CD | ARG | 245 | 25.919 | 82.937 | -17.270 | 1.00 | 39.75 | A |
| | ATOM | 936 | NE | ARG | 245 | 26.703 | 83.246 | -16.071 | 1.00 | 32.46 | A |
| | ATOM | 937 | HE | ARG | 245 | 26.520 | 82.731 | -15.258 | 1.00 | 0.00 | A |
| | ATOM | 938 | CZ | ARG | 245 | 27.636 | 84.192 | -16.014 | 1.00 | 34.10 | A |
| 55 | ATOM | 939 | NH1 | ARG | 245 | 27.911 | 84.933 | -17.085 | 1.00 | 32.74 | A |
| | ATOM | 940 | HH11 | ARG | 245 | 27.400 | 84.791 | -17.934 | 1.00 | 0.00 | A |
| | ATOM | 941 | HH12 | ARG | 245 | 28.616 | 85.640 | -17.039 | 1.00 | 0.00 | A |
| | ATOM | 942 | NH2 | ARG | 245 | 28.304 | 84.397 | -14.887 | 1.00 | 31.28 | A |
| | ATOM | 943 | HH21 | ARG | 245 | 28.098 | 83.847 | -14.077 | 1.00 | 0.00 | A |
| 60 | ATOM | 944 | HH22 | ARG | 245 | 29.009 | 85.102 | -14.847 | 1.00 | 0.00 | A |
| | ATOM | 945 | C | ARG | 245 | 26.366 | 77.868 | -16.937 | 1.00 | 37.43 | A |
| | ATOM | 946 | O | ARG | 245 | 27.190 | 77.640 | -16.053 | 1.00 | 32.06 | A |
| | ATOM | 947 | N | ARG | 246 | 26.243 | 77.120 | -18.030 | 1.00 | 36.45 | A |
| | ATOM | 948 | H | ARG | 246 | 25.576 | 77.378 | -18.700 | 1.00 | 0.00 | A |
| 65 | ATOM | 949 | CA | ARG | 246 | 27.052 | 75.931 | -18.279 | 1.00 | 40.85 | A |
| | ATOM | 950 | CB | ARG | 246 | 26.710 | 75.351 | -19.655 | 1.00 | 47.81 | A |
| | ATOM | 951 | CG | ARG | 246 | 25.360 | 74.674 | -19.728 | 1.00 | 56.42 | A |
| | ATOM | 952 | CD | ARG | 246 | 25.331 | 73.599 | -20.805 | 1.00 | 65.18 | A |
| | ATOM | 953 | NE | ARG | 246 | 24.144 | 72.756 | -20.688 | 1.00 | 70.92 | A |
| 70 | ATOM | 954 | HE | ARG | 246 | 23.939 | 72.373 | -19.811 | 1.00 | 0.00 | A |
| | ATOM | 955 | CZ | ARG | 246 | 23.324 | 72.473 | -21.697 | 1.00 | 75.61 | A |
| | ATOM | 956 | NH1 | ARG | 246 | 22.267 | 71.694 | -21.494 | 1.00 | 75.32 | A |
| | ATOM | 957 | HH11 | ARG | 246 | 22.087 | 71.323 | -20.583 | 1.00 | 0.00 | A |

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|----|------|-----|------|-----|-----|--------|--------|---------|------|-------|---|
| 5 | ATOM | 958 | HH12 | ARG | 246 | 21.650 | 71.482 | -22.252 | 1.00 | 0.00 | A |
| | ATOM | 959 | NH2 | ARG | 246 | 23.561 | 72.966 | -22.908 | 1.00 | 76.75 | A |
| | ATOM | 960 | HH21 | ARG | 246 | 24.357 | 73.550 | -23.064 | 1.00 | 0.00 | A |
| | ATOM | 961 | HH22 | ARG | 246 | 22.943 | 72.750 | -23.664 | 1.00 | 0.00 | A |
| | ATOM | 962 | C | ARG | 246 | 28.557 | 76.143 | -18.200 | 1.00 | 37.90 | A |
| 10 | ATOM | 963 | O | ARG | 246 | 29.149 | 76.779 | -19.074 | 1.00 | 41.30 | A |
| | ATOM | 964 | N | GLY | 247 | 29.172 | 75.602 | -17.157 | 1.00 | 30.93 | A |
| | ATOM | 965 | H | GLY | 247 | 28.658 | 75.119 | -16.478 | 1.00 | 0.00 | A |
| | ATOM | 966 | CA | GLY | 247 | 30.610 | 75.728 | -17.019 | 1.00 | 33.39 | A |
| | ATOM | 967 | C | GLY | 247 | 31.104 | 77.062 | -16.515 | 1.00 | 34.40 | A |
| 15 | ATOM | 968 | O | GLY | 247 | 32.280 | 77.394 | -16.648 | 1.00 | 37.30 | A |
| | ATOM | 969 | N | VAL | 248 | 30.206 | 77.853 | -15.947 | 1.00 | 37.33 | A |
| | ATOM | 970 | H | VAL | 248 | 29.266 | 77.576 | -15.906 | 1.00 | 0.00 | A |
| | ATOM | 971 | CA | VAL | 248 | 30.617 | 79.126 | -15.390 | 1.00 | 33.83 | A |
| | ATOM | 972 | CB | VAL | 248 | 29.506 | 80.168 | -15.526 | 1.00 | 29.27 | A |
| 20 | ATOM | 973 | CG1 | VAL | 248 | 29.660 | 81.239 | -14.471 | 1.00 | 27.00 | A |
| | ATOM | 974 | CG2 | VAL | 248 | 29.559 | 80.764 | -16.916 | 1.00 | 18.63 | A |
| | ATOM | 975 | C | VAL | 248 | 30.905 | 78.819 | -13.926 | 1.00 | 38.78 | A |
| | ATOM | 976 | O | VAL | 248 | 30.175 | 78.050 | -13.296 | 1.00 | 44.51 | A |
| | ATOM | 977 | N | LYS | 249 | 31.985 | 79.384 | -13.397 | 1.00 | 37.56 | A |
| 25 | ATOM | 978 | H | LYS | 249 | 32.536 | 79.980 | -13.946 | 1.00 | 0.00 | A |
| | ATOM | 979 | CA | LYS | 249 | 32.362 | 79.135 | -12.012 | 1.00 | 39.22 | A |
| | ATOM | 980 | CB | LYS | 249 | 33.644 | 79.894 | -11.660 | 1.00 | 42.55 | A |
| | ATOM | 981 | CG | LYS | 249 | 34.192 | 79.585 | -10.262 | 1.00 | 49.76 | A |
| | ATOM | 982 | CD | LYS | 249 | 34.281 | 78.082 | -9.992 | 1.00 | 50.58 | A |
| 30 | ATOM | 983 | CE | LYS | 249 | 34.354 | 77.781 | -8.498 | 1.00 | 53.51 | A |
| | ATOM | 984 | NZ | LYS | 249 | 35.759 | 77.621 | -8.011 | 1.00 | 56.75 | A |
| | ATOM | 985 | HZ1 | LYS | 249 | 36.289 | 78.498 | -8.188 | 1.00 | 0.00 | A |
| | ATOM | 986 | HZ2 | LYS | 249 | 36.213 | 76.834 | -8.518 | 1.00 | 0.00 | A |
| | ATOM | 987 | HZ3 | LYS | 249 | 35.752 | 77.418 | -6.992 | 1.00 | 0.00 | A |
| 35 | ATOM | 988 | C | LYS | 249 | 31.250 | 79.519 | -11.045 | 1.00 | 37.78 | A |
| | ATOM | 989 | O | LYS | 249 | 30.689 | 80.614 | -11.120 | 1.00 | 39.09 | A |
| | ATOM | 990 | N | LYS | 250 | 30.934 | 78.602 | -10.140 | 1.00 | 34.03 | A |
| | ATOM | 991 | H | LYS | 250 | 31.418 | 77.750 | -10.132 | 1.00 | 0.00 | A |
| | ATOM | 992 | CA | LYS | 250 | 29.888 | 78.833 | -9.161 | 1.00 | 33.73 | A |
| 40 | ATOM | 993 | CB | LYS | 250 | 29.116 | 77.537 | -8.890 | 1.00 | 32.39 | A |
| | ATOM | 994 | CG | LYS | 250 | 28.185 | 77.111 | -10.006 | 1.00 | 30.52 | A |
| | ATOM | 995 | CD | LYS | 250 | 28.424 | 75.659 | -10.376 | 1.00 | 33.84 | A |
| | ATOM | 996 | CE | LYS | 250 | 27.324 | 74.777 | -9.831 | 1.00 | 33.72 | A |
| | ATOM | 997 | NZ | LYS | 250 | 26.219 | 74.661 | -10.810 | 1.00 | 37.02 | A |
| 45 | ATOM | 998 | HZ1 | LYS | 250 | 26.577 | 74.247 | -11.692 | 1.00 | 0.00 | A |
| | ATOM | 999 | HZ2 | LYS | 250 | 25.828 | 75.607 | -11.003 | 1.00 | 0.00 | A |
| | ATOM | | | | | | | | | | |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1031 | CB | ILE | 254 | 26.933 | 81.416 | 3.476 | 1.00 | 26.55 | A |
| | ATOM | 1032 | CG2 | ILE | 254 | 25.851 | 81.144 | 4.512 | 1.00 | 23.36 | A |
| | ATOM | 1033 | CG1 | ILE | 254 | 26.764 | 80.415 | 2.330 | 1.00 | 23.69 | A |
| | ATOM | 1034 | CD1 | ILE | 254 | 28.047 | 79.781 | 1.869 | 1.00 | 23.22 | A |
| | ATOM | 1035 | C | ILE | 254 | 27.076 | 83.879 | 4.053 | 1.00 | 23.27 | A |
| | ATOM | 1036 | O | ILE | 254 | 28.222 | 84.121 | 4.418 | 1.00 | 26.33 | A |
| | ATOM | 1037 | N | VAL | 255 | 26.000 | 84.452 | 4.590 | 1.00 | 19.71 | A |
| 10 | ATOM | 1038 | H | VAL | 255 | 25.120 | 84.171 | 4.270 | 1.00 | 0.00 | A |
| | ATOM | 1039 | CA | VAL | 255 | 26.059 | 85.474 | 5.631 | 1.00 | 18.36 | A |
| | ATOM | 1040 | CB | VAL | 255 | 25.492 | 86.818 | 5.063 | 1.00 | 19.62 | A |
| | ATOM | 1041 | CG1 | VAL | 255 | 25.599 | 87.923 | 6.080 | 1.00 | 17.22 | A |
| 15 | ATOM | 1042 | CG2 | VAL | 255 | 26.254 | 87.209 | 3.790 | 1.00 | 20.74 | A |
| | ATOM | 1043 | C | VAL | 255 | 25.220 | 84.990 | 6.812 | 1.00 | 16.43 | A |
| | ATOM | 1044 | O | VAL | 255 | 24.035 | 84.701 | 6.649 | 1.00 | 19.58 | A |
| | ATOM | 1045 | N | THR | 256 | 25.826 | 84.875 | 7.990 | 1.00 | 15.49 | A |
| | ATOM | 1046 | H | THR | 256 | 26.770 | 85.121 | 8.082 | 1.00 | 0.00 | A |
| 20 | ATOM | 1047 | CA | THR | 256 | 25.084 | 84.390 | 9.142 | 1.00 | 14.90 | A |
| | ATOM | 1048 | CB | THR | 256 | 25.113 | 82.858 | 9.212 | 1.00 | 14.75 | A |
| | ATOM | 1049 | OG1 | THR | 256 | 24.240 | 82.400 | 10.253 | 1.00 | 13.11 | A |
| | ATOM | 1050 | HG1 | THR | 256 | 24.525 | 82.758 | 11.096 | 1.00 | 0.00 | A |
| | ATOM | 1051 | CG2 | THR | 256 | 26.526 | 82.378 | 9.476 | 1.00 | 12.09 | A |
| 25 | ATOM | 1052 | C | THR | 256 | 25.501 | 84.938 | 10.494 | 1.00 | 20.05 | A |
| | ATOM | 1053 | O | THR | 256 | 26.661 | 85.291 | 10.724 | 1.00 | 16.01 | A |
| | ATOM | 1054 | N | ASP | 257 | 24.512 | 84.930 | 11.385 | 1.00 | 21.65 | A |
| | ATOM | 1055 | H | ASP | 257 | 23.664 | 84.542 | 11.090 | 1.00 | 0.00 | A |
| | ATOM | 1056 | CA | ASP | 257 | 24.557 | 85.440 | 12.757 | 1.00 | 24.04 | A |
| 30 | ATOM | 1057 | CB | ASP | 257 | 23.199 | 86.096 | 13.031 | 1.00 | 29.68 | A |
| | ATOM | 1058 | CG | ASP | 257 | 23.297 | 87.308 | 13.891 | 1.00 | 38.27 | A |
| | ATOM | 1059 | OD1 | ASP | 257 | 24.426 | 87.791 | 14.137 | 1.00 | 52.10 | A |
| | ATOM | 1060 | OD2 | ASP | 257 | 22.228 | 87.780 | 14.321 | 1.00 | 36.38 | A |
| | ATOM | 1061 | C | ASP | 257 | 24.831 | 84.444 | 13.904 | 1.00 | 16.57 | A |
| 35 | ATOM | 1062 | O | ASP | 257 | 25.087 | 84.859 | 15.036 | 1.00 | 15.92 | A |
| | ATOM | 1063 | N | GLY | 258 | 24.731 | 83.150 | 13.643 | 1.00 | 12.93 | A |
| | ATOM | 1064 | H | GLY | 258 | 24.516 | 82.837 | 12.744 | 1.00 | 0.00 | A |
| | ATOM | 1065 | CA | GLY | 258 | 24.950 | 82.198 | 14.721 | 1.00 | 16.21 | A |
| | ATOM | 1066 | C | GLY | 258 | 25.155 | 80.786 | 14.229 | 1.00 | 21.42 | A |
| 40 | ATOM | 1067 | O | GLY | 258 | 25.226 | 80.552 | 13.026 | 1.00 | 16.78 | A |
| | ATOM | 1068 | N | GLU | 259 | 25.254 | 79.845 | 15.167 | 1.00 | 21.61 | A |
| | ATOM | 1069 | H | GLU | 259 | 25.190 | 80.105 | 16.110 | 1.00 | 0.00 | A |
| | ATOM | 1070 | CA | GLU | 259 | 25.450 | 78.442 | 14.832 | 1.00 | 22.54 | A |
| | ATOM | 1071 | CB | GLU | 259 | 25.801 | 77.649 | 16.093 | 1.00 | 27.50 | A |
| 45 | ATOM | 1072 | CG | GLU | 259 | 26.886 | 78.305 | 16.911 | 1.00 | 38.06 | A |
| | ATOM | 1073 | CD | GLU | 259 | 27.536 | 77.361 | 17.891 | 1.00 | 39.46 | A |
| | ATOM | 1074 | OE1 | GLU | 259 | 28.417 | 76.578 | 17.468 | 1.00 | 44.28 | A |
| | ATOM | 1075 | OE2 | GLU | 259 | 27.167 | 77.410 | 19.083 | 1.00 | 40.01 | A |
| | ATOM | 1076 | C | GLU | 259 | 24.196 | 77.875 | 14.187 | 1.00 | 19.71 | A |
| 50 | ATOM | 1077 | O | GLU | 259 | 23.093 | 78.316 | 14.468 | 1.00 | 16.96 | A |
| | ATOM | 1078 | N | SER | 260 | 24.357 | 76.886 | 13.324 | 1.00 | 21.81 | A |
| | ATOM | 1079 | H | SER | 260 | 25.252 | 76.526 | 13.145 | 1.00 | 0.00 | A |
| | ATOM | 1080 | CA | SER | 260 | 23.197 | 76.337 | 12.649 | 1.00 | 24.30 | A |
| | ATOM | 1081 | CB | SER | 260 | 23.585 | 75.761 | 11.287 | 1.00 | 26.30 | A |
| 55 | ATOM | 1082 | OG | SER | 260 | 24.643 | 74.827 | 11.404 | 1.00 | 27.86 | A |
| | ATOM | 1083 | HG | SER | 260 | 25.412 | 75.260 | 11.780 | 1.00 | 0.00 | A |
| | ATOM | 1084 | C | SER | 260 | 22.492 | 75.279 | 13.456 | 1.00 | 24.11 | A |
| | ATOM | 1085 | O | SER | 260 | 23.123 | 74.488 | 14.150 | 1.00 | 19.93 | A |
| | ATOM | 1086 | N | HIS | 261 | 21.166 | 75.303 | 13.384 | 1.00 | 30.37 | A |
| 60 | ATOM | 1087 | H | HIS | 261 | 20.726 | 76.006 | 12.864 | 1.00 | 0.00 | A |
| | ATOM | 1088 | CA | HIS | 261 | 20.352 | 74.308 | 14.062 | 1.00 | 35.00 | A |
| | ATOM | 1089 | CB | HIS | 261 | 18.862 | 74.616 | 13.876 | 1.00 | 38.14 | A |
| | ATOM | 1090 | CG | HIS | 261 | 18.263 | 75.417 | 14.994 | 1.00 | 40.87 | A |
| | ATOM | 1091 | CD2 | HIS | 261 | 17.159 | 75.203 | 15.749 | 1.00 | 38.31 | A |
| 65 | ATOM | 1092 | ND1 | HIS | 261 | 18.809 | 76.600 | 15.444 | 1.00 | 42.06 | A |
| | ATOM | 1093 | HD1 | HIS | 261 | 19.620 | 77.019 | 15.088 | 1.00 | 0.00 | A |
| | ATOM | 1094 | CE1 | HIS | 261 | 18.071 | 77.080 | 16.425 | 1.00 | 41.84 | A |
| | ATOM | 1095 | NE2 | HIS | 261 | 17.062 | 76.251 | 16.631 | 1.00 | 38.37 | A |
| | ATOM | 1096 | HE2 | HIS | 261 | 16.358 | 76.361 | 17.297 | 1.00 | 0.00 | A |
| 70 | ATOM | 1097 | C | HIS | 261 | 20.715 | 73.032 | 13.316 | 1.00 | 36.08 | A |
| | ATOM | 1098 | O | HIS | 261 | 20.886 | 71.969 | 13.915 | 1.00 | 32.42 | A |
| | ATOM | 1099 | N | TYR | 262 | 20.857 | 73.173 | 11.997 | 1.00 | 39.63 | A |
| | ATOM | 1100 | H | TYR | 262 | 20.705 | 74.056 | 11.602 | 1.00 | 0.00 | A |
| | ATOM | 1101 | CA | TYR | 262 | 21.224 | 72.069 | 11.122 | 1.00 | 45.92 | A |
| | ATOM | 1102 | CB | TYR | 262 | 20.783 | 72.372 | 9.689 | 1.00 | 52.25 | A |
| | ATOM | 1103 | CG | TYR | 262 | 19.879 | 71.310 | 9.137 | 1.00 | 62.19 | A |

| | | | | | | | | | | | |
|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| | ATOM | 1104 | CD1 | TYR | 262 | 19.511 | 71.302 | 7.792 | 1.00 | 67.63 | A |
| | ATOM | 1105 | CE1 | TYR | 262 | 18.676 | 70.297 | 7.280 | 1.00 | 69.78 | A |
| | ATOM | 1106 | CD2 | TYR | 262 | 19.398 | 70.290 | 9.960 | 1.00 | 66.65 | A |
| 5 | ATOM | 1107 | CE2 | TYR | 262 | 18.569 | 69.285 | 9.465 | 1.00 | 69.62 | A |
| | ATOM | 1108 | CZ | TYR | 262 | 18.213 | 69.290 | 8.125 | 1.00 | 71.57 | A |
| | ATOM | 1109 | OH | TYR | 262 | 17.408 | 68.282 | 7.637 | 1.00 | 70.23 | A |
| | ATOM | 1110 | HH | TYR | 262 | 17.185 | 67.678 | 8.350 | 1.00 | 0.00 | A |
| | ATOM | 1111 | C | TYR | 262 | 22.728 | 71.793 | 11.152 | 1.00 | 45.91 | A |
| 10 | ATOM | 1112 | O | TYR | 262 | 23.270 | 71.219 | 10.215 | 1.00 | 45.20 | A |
| | ATOM | 1113 | N | ASN | 263 | 23.377 | 72.230 | 12.233 | 1.00 | 47.51 | A |
| | ATOM | 1114 | H | ASN | 263 | 22.849 | 72.702 | 12.906 | 1.00 | 0.00 | A |
| | ATOM | 1115 | CA | ASN | 263 | 24.817 | 72.066 | 12.500 | 1.00 | 47.67 | A |
| | ATOM | 1116 | CB | ASN | 263 | 25.022 | 71.886 | 14.011 | 1.00 | 49.01 | A |
| 15 | ATOM | 1117 | CG | ASN | 263 | 26.334 | 72.466 | 14.504 | 1.00 | 54.05 | A |
| | ATOM | 1118 | OD1 | ASN | 263 | 27.373 | 71.805 | 14.449 | 1.00 | 54.43 | A |
| | ATOM | 1119 | ND2 | ASN | 263 | 26.290 | 73.702 | 15.000 | 1.00 | 47.01 | A |
| | ATOM | 1120 | HD21 | ASN | 263 | 25.440 | 74.188 | 15.032 | 1.00 | 0.00 | A |
| | ATOM | 1121 | HD22 | ASN | 263 | 27.130 | 74.088 | 15.322 | 1.00 | 0.00 | A |
| 20 | ATOM | 1122 | C | ASN | 263 | 25.434 | 70.873 | 11.775 | 1.00 | 49.23 | A |
| | ATOM | 1123 | O | ASN | 263 | 26.273 | 71.026 | 10.881 | 1.00 | 46.48 | A |
| | ATOM | 1124 | N | HIS | 264 | 25.029 | 69.681 | 12.197 | 1.00 | 48.43 | A |
| | ATOM | 1125 | H | HIS | 264 | 24.391 | 69.635 | 12.939 | 1.00 | 0.00 | A |
| | ATOM | 1126 | CA | HIS | 264 | 25.496 | 68.439 | 11.599 | 1.00 | 47.59 | A |
| 25 | ATOM | 1127 | CB | HIS | 264 | 24.755 | 67.255 | 12.228 | 1.00 | 46.90 | A |
| | ATOM | 1128 | CG | HIS | 264 | 23.275 | 67.462 | 12.359 | 1.00 | 50.04 | A |
| | ATOM | 1129 | CD2 | HIS | 264 | 22.549 | 68.207 | 13.229 | 1.00 | 53.97 | A |
| | ATOM | 1130 | ND1 | HIS | 264 | 22.360 | 66.865 | 11.517 | 1.00 | 51.14 | A |
| | ATOM | 1131 | HD1 | HIS | 264 | 22.581 | 66.256 | 10.788 | 1.00 | 0.00 | A |
| 30 | ATOM | 1132 | CE1 | HIS | 264 | 21.138 | 67.228 | 11.864 | 1.00 | 53.11 | A |
| | ATOM | 1133 | NE2 | HIS | 264 | 21.225 | 68.044 | 12.898 | 1.00 | 55.29 | A |
| | ATOM | 1134 | HE2 | HIS | 264 | 20.471 | 68.460 | 13.361 | 1.00 | 0.00 | A |
| | ATOM | 1135 | C | HIS | 264 | 25.132 | 68.550 | 10.130 | 1.00 | 46.97 | A |
| | ATOM | 1136 | O | HIS | 264 | 24.666 | 69.593 | 9.686 | 1.00 | 51.57 | A |
| 35 | ATOM | 1137 | N | ARG | 265 | 25.348 | 67.496 | 9.358 | 1.00 | 44.23 | A |
| | ATOM | 1138 | H | ARG | 265 | 25.749 | 66.684 | 9.732 | 1.00 | 0.00 | A |
| | ATOM | 1139 | CA | ARG | 265 | 24.983 | 67.554 | 7.946 | 1.00 | 41.47 | A |
| | ATOM | 1140 | CB | ARG | 265 | 23.473 | 67.816 | 7.831 | 1.00 | 40.64 | A |
| | ATOM | 1141 | CG | ARG | 265 | 23.030 | 68.564 | 6.591 | 1.00 | 43.80 | A |
| 40 | ATOM | 1142 | CD | ARG | 265 | 21.666 | 68.091 | 6.130 | 1.00 | 47.91 | A |
| | ATOM | 1143 | NE | ARG | 265 | 21.163 | 68.876 | 5.005 | 1.00 | 56.53 | A |
| | ATOM | 1144 | HE | ARG | 265 | 21.797 | 69.449 | 4.527 | 1.00 | 0.00 | A |
| | ATOM | 1145 | CZ | ARG | 265 | 19.901 | 68.861 | 4.588 | 1.00 | 58.89 | A |
| | ATOM | 1146 | NH1 | ARG | 265 | 19.006 | 68.099 | 5.202 | 1.00 | 64.72 | A |
| 45 | ATOM | 1147 | HH11 | ARG | 265 | 19.281 | 67.532 | 5.979 | 1.00 | 0.00 | A |
| | ATOM | 1148 | HH12 | ARG | 265 | 18.057 | 68.088 | 4.887 | 1.00 | 0.00 | A |
| | ATOM | 1149 | NH2 | ARG | 265 | 19.530 | 69.612 | 3.561 | 1.00 | 63.20 | A |
| | ATOM | 1150 | HH21 | ARG | 265 | 20.200 | 70.192 | 3.097 | 1.00 | 0.00 | A |
| | ATOM | 1151 | HH22 | ARG | 265 | 18.580 | 69.600 | 3.250 | 1.00 | 0.00 | A |
| 50 | ATOM | 1152 | C | ARG | 265 | 25.777 | 68.622 | 7.176 | 1.00 | 37.16 | A |
| | ATOM | 1153 | O | ARG | 265 | 25.768 | 68.641 | 5.943 | 1.00 | 37.73 | A |
| | ATOM | 1154 | N | LEU | 266 | 26.466 | 69.497 | 7.904 | 1.00 | 30.79 | A |
| | ATOM | 1155 | H | LEU | 266 | 26.433 | 69.434 | 8.878 | 1.00 | 0.00 | A |
| | ATOM | 1156 | CA | LEU | 266 | 27.274 | 70.551 | 7.290 | 1.00 | 37.31 | A |
| 55 | ATOM | 1157 | CB | LEU | 266 | 27.832 | 71.482 | 8.368 | 1.00 | 31.59 | A |
| | ATOM | 1158 | CG | LEU | 266 | 27.685 | 73.002 | 8.258 | 1.00 | 31.43 | A |
| | ATOM | 1159 | CD1 | LEU | 266 | 26.593 | 73.400 | 7.273 | 1.00 | 36.39 | A |
| | ATOM | 1160 | CD2 | LEU | 266 | 27.383 | 73.540 | 9.638 | 1.00 | 28.41 | A |
| | ATOM | 1161 | C | LEU | 266 | 28.430 | 69.925 | 6.523 | 1.00 | 42.12 | A |
| 60 | ATOM | 1162 | O | LEU | 266 | 28.719 | 70.299 | 5.388 | 1.00 | 43.04 | A |
| | ATOM | 1163 | N | GLN | 267 | 29.091 | 68.967 | 7.164 | 1.00 | 46.26 | A |
| | ATOM | 1164 | H | GLN | 267 | 28.809 | 68.723 | 8.070 | 1.00 | 0.00 | A |
| | ATOM | 1165 | CA | GLN | 267 | 30.218 | 68.269 | 6.567 | 1.00 | 48.62 | A |
| | ATOM | 1166 | CB | GLN | 267 | 30.721 | 67.188 | 7.521 | 1.00 | 54.56 | A |
| 65 | ATOM | 1167 | CG | GLN | 267 | 30.666 | 67.601 | 8.987 | 1.00 | 62.75 | A |
| | ATOM | 1168 | CD | GLN | 267 | 31.869 | 67.127 | 9.787 | 1.00 | 67.47 | A |
| | ATOM | 1169 | OE1 | GLN | 267 | 32.730 | 66.406 | 9.273 | 1.00 | 71.87 | A |
| | ATOM | 1170 | NE2 | GLN | 267 | 31.935 | 67.527 | 11.055 | 1.00 | 68.16 | A |
| | ATOM | 1171 | HE21 | GLN | 267 | 31.227 | 68.098 | 11.420 | 1.00 | 0.00 | A |
| 70 | ATOM | 1172 | HE22 | GLN | 267 | 32.700 | 67.231 | 11.584 | 1.00 | 0.00 | A |
| | ATOM | 1173 | C | GLN | 267 | 29.830 | 67.649 | 5.231 | 1.00 | 48.74 | A |
| | ATOM | 1174 | O | GLN | 267 | 30.597 | 67.700 | 4.271 | 1.00 | 47.96 | A |
| | ATOM | 1175 | N | LYS | 268 | 28.637 | 67.067 | 5.166 | 1.00 | 45.46 | A |
| | ATOM | 1176 | H | LYS | 268 | 28.058 | 67.047 | 5.955 | 1.00 | 0.00 | A |

| | | | | | | | | | | | |
|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1177 | CA | LYS | 268 | 28.191 | 66.463 | 3.924 | 1.00 | 45.48 | A |
| | ATOM | 1178 | CB | LYS | 268 | 27.048 | 65.477 | 4.181 | 1.00 | 49.81 | A |
| | ATOM | 1179 | CG | LYS | 268 | 27.042 | 64.279 | 3.240 | 1.00 | 56.67 | A |
| | ATOM | 1180 | CD | LYS | 268 | 28.157 | 63.290 | 3.578 | 1.00 | 61.88 | A |
| | ATOM | 1181 | CE | LYS | 268 | 29.009 | 62.946 | 2.354 | 1.00 | 64.81 | A |
| 10 | ATOM | 1182 | NZ | LYS | 268 | 29.927 | 61.787 | 2.599 | 1.00 | 70.64 | A |
| | ATOM | 1183 | HZ1 | LYS | 268 | 29.368 | 60.945 | 2.844 | 1.00 | 0.00 | A |
| | ATOM | 1184 | HZ2 | LYS | 268 | 30.573 | 62.014 | 3.383 | 1.00 | 0.00 | A |
| | ATOM | 1185 | HZ3 | LYS | 268 | 30.482 | 61.595 | 1.740 | 1.00 | 0.00 | A |
| | ATOM | 1186 | C | LYS | 268 | 27.744 | 67.533 | 2.939 | 1.00 | 40.50 | A |
| 15 | ATOM | 1187 | O | LYS | 268 | 27.960 | 67.402 | 1.742 | 1.00 | 40.62 | A |
| | ATOM | 1188 | N | VAL | 269 | 27.133 | 68.603 | 3.434 | 1.00 | 39.04 | A |
| | ATOM | 1189 | H | VAL | 269 | 26.991 | 68.684 | 4.400 | 1.00 | 0.00 | A |
| | ATOM | 1190 | CA | VAL | 269 | 26.676 | 69.663 | 2.538 | 1.00 | 37.29 | A |
| | ATOM | 1191 | CB | VAL | 269 | 25.782 | 70.685 | 3.269 | 1.00 | 34.20 | A |
| 20 | ATOM | 1192 | CG1 | VAL | 269 | 25.492 | 71.860 | 2.356 | 1.00 | 29.69 | A |
| | ATOM | 1193 | CG2 | VAL | 269 | 24.492 | 70.026 | 3.703 | 1.00 | 31.32 | A |
| | ATOM | 1194 | C | VAL | 269 | 27.857 | 70.404 | 1.921 | 1.00 | 35.64 | A |
| | ATOM | 1195 | O | VAL | 269 | 27.844 | 70.725 | 0.734 | 1.00 | 37.28 | A |
| | ATOM | 1196 | N | ILE | 270 | 28.876 | 70.667 | 2.731 | 1.00 | 31.83 | A |
| 25 | ATOM | 1197 | H | ILE | 270 | 28.833 | 70.374 | 3.661 | 1.00 | 0.00 | A |
| | ATOM | 1198 | CA | ILE | 270 | 30.052 | 71.375 | 2.261 | 1.00 | 33.15 | A |
| | ATOM | 1199 | CB | ILE | 270 | 30.971 | 71.750 | 3.438 | 1.00 | 33.05 | A |
| | ATOM | 1200 | CG2 | ILE | 270 | 32.222 | 72.469 | 2.930 | 1.00 | 24.49 | A |
| | ATOM | 1201 | CG1 | ILE | 270 | 30.209 | 72.643 | 4.417 | 1.00 | 29.68 | A |
| 30 | ATOM | 1202 | CD1 | ILE | 270 | 30.041 | 74.059 | 3.944 | 1.00 | 32.31 | A |
| | ATOM | 1203 | C | ILE | 270 | 30.835 | 70.541 | 1.252 | 1.00 | 38.00 | A |
| | ATOM | 1204 | O | ILE | 270 | 31.190 | 71.026 | 0.176 | 1.00 | 34.89 | A |
| | ATOM | 1205 | N | GLN | 271 | 31.092 | 69.283 | 1.603 | 1.00 | 37.30 | A |
| | ATOM | 1206 | H | GLN | 271 | 30.776 | 68.956 | 2.471 | 1.00 | 0.00 | A |
| 35 | ATOM | 1207 | CA | GLN | 271 | 31.836 | 68.378 | 0.735 | 1.00 | 40.28 | A |
| | ATOM | 1208 | CB | GLN | 271 | 32.061 | 67.038 | 1.442 | 1.00 | 45.96 | A |
| | ATOM | 1209 | CG | GLN | 271 | 32.724 | 65.972 | 0.580 | 1.00 | 50.37 | A |
| | ATOM | 1210 | CD | GLN | 271 | 34.111 | 66.365 | 0.114 | 1.00 | 54.51 | A |
| | ATOM | 1211 | OE1 | GLN | 271 | 34.298 | 66.806 | -1.026 | 1.00 | 54.16 | A |
| 40 | ATOM | 1212 | NE2 | GLN | 271 | 35.102 | 66.201 | 0.988 | 1.00 | 55.62 | A |
| | ATOM | 1213 | HE21 | GLN | 271 | 34.908 | 65.841 | 1.879 | 1.00 | 0.00 | A |
| | ATOM | 1214 | HE22 | GLN | 271 | 36.004 | 66.448 | 0.704 | 1.00 | 0.00 | A |
| | ATOM | 1215 | C | GLN | 271 | 31.103 | 68.154 | -0.583 | 1.00 | 42.88 | A |
| | ATOM | 1216 | O | GLN | 271 | 31.722 | 67.846 | -1.599 | 1.00 | 46.33 | A |
| 45 | ATOM | 1217 | N | ASP | 272 | 29.783 | 68.297 | -0.566 | 1.00 | 40.17 | A |
| | ATOM | 1218 | H | ASP | 272 | 29.330 | 68.520 | 0.276 | 1.00 | 0.00 | A |
| | ATOM | 1219 | CA | ASP | 272 | 28.999 | 68.125 | -1.778 | 1.00 | 41.34 | A |
| | ATOM | 1220 | CB | ASP | 272 | 27.529 | 67.885 | -1.439 | 1.00 | 43.85 | A |
| | ATOM | 1221 | CG | ASP | 272 | 27.249 | 66.451 | -1.068 | 1.00 | 45.57 | A |
| 50 | ATOM | 1222 | OD1 | ASP | 272 | 27.395 | 66.103 | 0.115 | 1.00 | 46.69 | A |
| | ATOM | 1223 | OD2 | ASP | 272 | 26.885 | 65.663 | -1.960 | 1.00 | 53.57 | A |
| | ATOM | 1224 | C | ASP | 272 | 29.128 | 69.379 | -2.632 | 1.00 | 41.62 | A |
| | ATOM | 1225 | O | ASP | 272 | 28.871 | 69.354 | -3.841 | 1.00 | 39.28 | A |
| | ATOM | 1226 | N | CYS | 273 | 29.520 | 70.477 | -1.992 | 1.00 | 37.21 | A |
| 55 | ATOM | 1227 | H | CYS | 273 | 29.694 | 70.431 | -1.028 | 1.00 | 0.00 | A |
| | ATOM | 1228 | CA | CYS | 273 | 29.697 | 71.746 | -2.685 | 1.00 | 34.88 | A |
| | ATOM | 1229 | CB | CYS | 273 | 29.580 | 72.910 | -1.697 | 1.00 | 28.59 | A |
| | ATOM | 1230 | SG | CYS | 273 | 27.871 | 73.342 | -1.278 | 1.00 | 31.88 | A |
| | ATOM | 1231 | C | CYS | 273 | 31.078 | 71.760 | -3.326 | 1.00 | 34.92 | A |
| 60 | ATOM | 1232 | O | CYS | 273 | 31.226 | 72.094 | -4.504 | 1.00 | 26.50 | A |
| | ATOM | 1233 | N | GLU | 274 | 32.072 | 71.384 | -2.524 | 1.00 | 35.57 | A |
| | ATOM | 1234 | H | GLU | 274 | 31.847 | 71.129 | -1.606 | 1.00 | 0.00 | A |
| | ATOM | 1235 | CA | GLU | 274 | 33.470 | 71.329 | -2.924 | 1.00 | 38.47 | A |
| | ATOM | 1236 | CB | GLU | 274 | 34.305 | 70.927 | -1.706 | 1.00 | 45.16 | A |
| 65 | ATOM | 1237 | CG | GLU | 274 | 35.785 | 70.680 | -1.935 | 1.00 | 50.75 | A |
| | ATOM | 1238 | CD | GLU | 274 | 36.356 | 69.705 | -0.908 | 1.00 | 56.66 | A |
| | ATOM | 1239 | OE1 | GLU | 274 | 37.306 | 70.063 | -0.173 | 1.00 | 58.10 | A |
| | ATOM | 1240 | OE2 | GLU | 274 | 35.846 | 68.569 | -0.833 | 1.00 | 62.18 | A |
| | ATOM | 1241 | C | GLU | 274 | 33.629 | 70.318 | -4.054 | 1.00 | 43.44 | A |
| 70 | ATOM | 1242 | O | GLU | 274 | 34.555 | 70.407 | -4.862 | 1.00 | 46.62 | A |
| | ATOM | 1243 | N | ASP | 275 | 32.713 | 69.357 | -4.112 | 1.00 | 44.68 | A |
| | ATOM | 1244 | H | ASP | 275 | 32.002 | 69.326 | -3.440 | 1.00 | 0.00 | A |
| | ATOM | 1245 | CA | ASP | 275 | 32.757 | 68.356 | -5.160 | 1.00 | 43.67 | A |
| | ATOM | 1246 | CB | ASP | 275 | 31.995 | 67.104 | -4.737 | 1.00 | 48.36 | A |
| | ATOM | 1247 | CG | ASP | 275 | 32.919 | 65.936 | -4.468 | 1.00 | 49.82 | A |
| | ATOM | 1248 | OD1 | ASP | 275 | 32.936 | 64.992 | -5.286 | 1.00 | 54.38 | A |
| | ATOM | 1249 | OD2 | ASP | 275 | 33.634 | 65.969 | -3.443 | 1.00 | 54.23 | A |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1250 | C | ASP | 275 | 32.158 | 68.947 | -6.428 | 1.00 | 43.28 | A |
| | ATOM | 1251 | O | ASP | 275 | 32.578 | 68.610 | -7.540 | 1.00 | 35.41 | A |
| | ATOM | 1252 | N | GLU | 276 | 31.187 | 69.840 | -6.256 | 1.00 | 39.61 | A |
| | ATOM | 1253 | H | GLU | 276 | 30.890 | 70.058 | -5.349 | 1.00 | 0.00 | A |
| | ATOM | 1254 | CA | GLU | 276 | 30.551 | 70.503 | -7.392 | 1.00 | 42.30 | A |
| | ATOM | 1255 | CB | GLU | 276 | 29.085 | 70.815 | -7.078 | 1.00 | 44.73 | A |
| | ATOM | 1256 | CG | GLU | 276 | 28.246 | 69.581 | -6.784 | 1.00 | 47.48 | A |
| 10 | ATOM | 1257 | CD | GLU | 276 | 26.769 | 69.817 | -7.011 | 1.00 | 50.24 | A |
| | ATOM | 1258 | OE1 | GLU | 276 | 25.950 | 69.064 | -6.437 | 1.00 | 50.57 | A |
| | ATOM | 1259 | OE2 | GLU | 276 | 26.428 | 70.755 | -7.762 | 1.00 | 48.92 | A |
| 15 | ATOM | 1260 | C | GLU | 276 | 31.314 | 71.793 | -7.678 | 1.00 | 40.70 | A |
| | ATOM | 1261 | O | GLU | 276 | 30.789 | 72.716 | -8.301 | 1.00 | 40.89 | A |
| | ATOM | 1262 | N | ASN | 277 | 32.563 | 71.829 | -7.211 | 1.00 | 40.17 | A |
| | ATOM | 1263 | H | ASN | 277 | 32.899 | 71.045 | -6.732 | 1.00 | 0.00 | A |
| | ATOM | 1264 | CA | ASN | 277 | 33.465 | 72.974 | -7.373 | 1.00 | 40.38 | A |
| | ATOM | 1265 | CB | ASN | 277 | 34.157 | 72.914 | -8.733 | 1.00 | 41.95 | A |
| | ATOM | 1266 | CG | ASN | 277 | 35.220 | 71.832 | -8.789 | 1.00 | 47.84 | A |
| 20 | ATOM | 1267 | OD1 | ASN | 277 | 36.408 | 72.097 | -8.578 | 1.00 | 49.04 | A |
| | ATOM | 1268 | ND2 | ASN | 277 | 34.791 | 70.605 | -9.066 | 1.00 | 46.30 | A |
| | ATOM | 1269 | HD21 | ASN | 277 | 33.840 | 70.438 | -9.221 | 1.00 | 0.00 | A |
| | ATOM | 1270 | HD22 | ASN | 277 | 35.466 | 69.895 | -9.104 | 1.00 | 0.00 | A |
| 25 | ATOM | 1271 | C | ASN | 277 | 32.791 | 74.327 | -7.192 | 1.00 | 36.39 | A |
| | ATOM | 1272 | O | ASN | 277 | 32.712 | 75.137 | -8.119 | 1.00 | 36.27 | A |
| | ATOM | 1273 | N | ILE | 278 | 32.320 | 74.569 | -5.980 | 1.00 | 34.58 | A |
| | ATOM | 1274 | H | ILE | 278 | 32.422 | 73.890 | -5.281 | 1.00 | 0.00 | A |
| | ATOM | 1275 | CA | ILE | 278 | 31.652 | 75.819 | -5.665 | 1.00 | 34.26 | A |
| | ATOM | 1276 | CB | ILE | 278 | 30.228 | 75.549 | -5.162 | 1.00 | 30.91 | A |
| | ATOM | 1277 | CG2 | ILE | 278 | 29.646 | 76.814 | -4.530 | 1.00 | 32.30 | A |
| 30 | ATOM | 1278 | CG1 | ILE | 278 | 29.368 | 75.058 | -6.331 | 1.00 | 26.81 | A |
| | ATOM | 1279 | CD1 | ILE | 278 | 27.955 | 74.622 | -5.936 | 1.00 | 27.38 | A |
| | ATOM | 1280 | C | ILE | 278 | 32.424 | 76.617 | -4.616 | 1.00 | 35.39 | A |
| 35 | ATOM | 1281 | O | ILE | 278 | 32.412 | 76.275 | -3.431 | 1.00 | 35.14 | A |
| | ATOM | 1282 | N | GLN | 279 | 33.105 | 77.671 | -5.062 | 1.00 | 34.70 | A |
| | ATOM | 1283 | H | GLN | 279 | 33.095 | 77.872 | -6.022 | 1.00 | 0.00 | A |
| | ATOM | 1284 | CA | GLN | 279 | 33.869 | 78.537 | -4.166 | 1.00 | 33.01 | A |
| | ATOM | 1285 | CB | GLN | 279 | 34.560 | 79.647 | -4.954 | 1.00 | 38.07 | A |
| | ATOM | 1286 | CG | GLN | 279 | 35.956 | 79.282 | -5.430 | 1.00 | 46.02 | A |
| | ATOM | 1287 | CD | GLN | 279 | 37.019 | 80.222 | -4.886 | 1.00 | 49.56 | A |
| 40 | ATOM | 1288 | OE1 | GLN | 279 | 36.779 | 81.422 | -4.726 | 1.00 | 40.91 | A |
| | ATOM | 1289 | NE2 | GLN | 279 | 38.205 | 79.680 | -4.601 | 1.00 | 48.01 | A |
| | ATOM | 1290 | HE21 | GLN | 279 | 38.352 | 78.722 | -4.749 | 1.00 | 0.00 | A |
| 45 | ATOM | 1291 | HE22 | GLN | 279 | 38.901 | 80.273 | -4.252 | 1.00 | 0.00 | A |
| | ATOM | 1292 | C | GLN | 279 | 32.900 | 79.155 | -3.163 | 1.00 | 30.48 | A |
| | ATOM | 1293 | O | GLN | 279 | 31.861 | 79.680 | -3.543 | 1.00 | 26.66 | A |
| | ATOM | 1294 | N | ARG | 280 | 33.253 | 79.098 | -1.882 | 1.00 | 31.39 | A |
| | ATOM | 1295 | H | ARG | 280 | 34.114 | 78.698 | -1.641 | 1.00 | 0.00 | A |
| | ATOM | 1296 | CA | ARG | 280 | 32.388 | 79.622 | -0.833 | 1.00 | 32.62 | A |
| | ATOM | 1297 | CB | ARG | 280 | 31.864 | 78.452 | 0.013 | 1.00 | 31.05 | A |
| 50 | ATOM | 1298 | CG | ARG | 280 | 31.447 | 77.246 | -0.823 | 1.00 | 30.23 | A |
| | ATOM | 1299 | CD | ARG | 280 | 31.031 | 76.072 | 0.033 | 1.00 | 29.02 | A |
| | ATOM | 1300 | NE | ARG | 280 | 32.172 | 75.403 | 0.641 | 1.00 | 23.82 | A |
| 55 | ATOM | 1301 | HE | ARG | 280 | 32.358 | 75.574 | 1.588 | 1.00 | 0.00 | A |
| | ATOM | 1302 | CZ | ARG | 280 | 32.972 | 74.567 | -0.008 | 1.00 | 30.22 | A |
| | ATOM | 1303 | NH1 | ARG | 280 | 32.756 | 74.297 | -1.290 | 1.00 | 32.10 | A |
| | ATOM | 1304 | HH11 | ARG | 280 | 31.983 | 74.717 | -1.766 | 1.00 | 0.00 | A |
| | ATOM | 1305 | HH12 | ARG | 280 | 33.362 | 73.669 | -1.778 | 1.00 | 0.00 | A |
| | ATOM | 1306 | NH2 | ARG | 280 | 33.985 | 73.996 | 0.627 | 1.00 | 33.41 | A |
| | ATOM | 1307 | HH21 | ARG | 280 | 34.141 | 74.190 | 1.595 | 1.00 | 0.00 | A |
| 60 | ATOM | 1308 | HH22 | ARG | 280 | 34.592 | 73.369 | 0.138 | 1.00 | 0.00 | A |
| | ATOM | 1309 | C | ARG | 280 | 33.046 | 80.673 | 0.070 | 1.00 | 31.10 | A |
| | ATOM | 1310 | O | ARG | 280 | 34.146 | 80.477 | 0.598 | 1.00 | 29.04 | A |
| 65 | ATOM | 1311 | N | PHE | 281 | 32.354 | 81.792 | 0.231 | 1.00 | 27.75 | A |
| | ATOM | 1312 | H | PHE | 281 | 31.499 | 81.890 | -0.231 | 1.00 | 0.00 | A |
| | ATOM | 1313 | CA | PHE | 281 | 32.824 | 82.879 | 1.074 | 1.00 | 30.07 | A |
| | ATOM | 1314 | CB | PHE | 281 | 32.798 | 84.199 | 0.303 | 1.00 | 28.77 | A |
| | ATOM | 1315 | CG | PHE | 281 | 33.920 | 84.348 | -0.671 | 1.00 | 31.37 | A |
| | ATOM | 1316 | CD1 | PHE | 281 | 33.774 | 83.928 | -1.988 | 1.00 | 37.93 | A |
| | ATOM | 1317 | CD2 | PHE | 281 | 35.136 | 84.893 | -0.272 | 1.00 | 33.95 | A |
| 70 | ATOM | 1318 | CE1 | PHE | 281 | 34.830 | 84.047 | -2.894 | 1.00 | 38.18 | A |
| | ATOM | 1319 | CE2 | PHE | 281 | 36.196 | 85.014 | -1.174 | 1.00 | 31.36 | A |
| | ATOM | 1320 | CZ | PHE | 281 | 36.042 | 84.591 | -2.481 | 1.00 | 33.33 | A |
| | ATOM | 1321 | C | PHE | 281 | 31.857 | 82.952 | 2.247 | 1.00 | 31.00 | A |
| | ATOM | 1322 | O | PHE | 281 | 30.676 | 83.214 | 2.045 | 1.00 | 33.33 | A |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1323 | N | SER | 282 | 32.337 | 82.708 | 3.463 | 1.00 | 27.38 | A |
| | ATOM | 1324 | H | SER | 282 | 33.286 | 82.493 | 3.582 | 1.00 | 0.00 | A |
| | ATOM | 1325 | CA | SER | 282 | 31.455 | 82.765 | 4.610 | 1.00 | 31.18 | A |
| | ATOM | 1326 | CB | SER | 282 | 31.462 | 81.425 | 5.359 | 1.00 | 29.23 | A |
| | ATOM | 1327 | OG | SER | 282 | 32.690 | 81.189 | 6.020 | 1.00 | 25.15 | A |
| 10 | ATOM | 1328 | HG | SER | 282 | 33.402 | 81.171 | 5.376 | 1.00 | 0.00 | A |
| | ATOM | 1329 | C | SER | 282 | 31.777 | 83.919 | 5.560 | 1.00 | 32.76 | A |
| | ATOM | 1330 | O | SER | 282 | 32.886 | 84.044 | 6.079 | 1.00 | 37.88 | A |
| | ATOM | 1331 | N | ILE | 283 | 30.777 | 84.766 | 5.766 | 1.00 | 33.62 | A |
| | ATOM | 1332 | H | ILE | 283 | 29.927 | 84.603 | 5.308 | 1.00 | 0.00 | A |
| 15 | ATOM | 1333 | CA | ILE | 283 | 30.887 | 85.921 | 6.634 | 1.00 | 30.37 | A |
| | ATOM | 1334 | CB | ILE | 283 | 30.324 | 87.183 | 5.944 | 1.00 | 33.69 | A |
| | ATOM | 1335 | CG2 | ILE | 283 | 30.920 | 88.435 | 6.571 | 1.00 | 33.06 | A |
| | ATOM | 1336 | CG1 | ILE | 283 | 30.634 | 87.144 | 4.448 | 1.00 | 28.09 | A |
| | ATOM | 1337 | CD1 | ILE | 283 | 30.588 | 88.512 | 3.781 | 1.00 | 33.55 | A |
| 20 | ATOM | 1338 | C | ILE | 283 | 30.095 | 85.671 | 7.911 | 1.00 | 30.75 | A |
| | ATOM | 1339 | O | ILE | 283 | 28.878 | 85.485 | 7.869 | 1.00 | 30.38 | A |
| | ATOM | 1340 | N | ALA | 284 | 30.797 | 85.658 | 9.038 | 1.00 | 25.22 | A |
| | ATOM | 1341 | H | ALA | 284 | 31.767 | 85.785 | 8.990 | 1.00 | 0.00 | A |
| | ATOM | 1342 | CA | ALA | 284 | 30.183 | 85.462 | 10.344 | 1.00 | 25.92 | A |
| 25 | ATOM | 1343 | CB | ALA | 284 | 31.034 | 84.480 | 11.172 | 1.00 | 26.80 | A |
| | ATOM | 1344 | C | ALA | 284 | 30.026 | 86.790 | 11.114 | 1.00 | 25.45 | A |
| | ATOM | 1345 | O | ALA | 284 | 31.025 | 87.437 | 11.458 | 1.00 | 23.52 | A |
| | ATOM | 1346 | N | ILE | 285 | 28.780 | 87.188 | 11.379 | 1.00 | 21.71 | A |
| | ATOM | 1347 | H | ILE | 285 | 28.033 | 86.646 | 11.052 | 1.00 | 0.00 | A |
| 30 | ATOM | 1348 | CA | ILE | 285 | 28.484 | 88.404 | 12.142 | 1.00 | 14.56 | A |
| | ATOM | 1349 | CB | ILE | 285 | 27.122 | 89.033 | 11.672 | 1.00 | 20.57 | A |
| | ATOM | 1350 | CG2 | ILE | 285 | 26.861 | 90.366 | 12.360 | 1.00 | 16.36 | A |
| | ATOM | 1351 | CG1 | ILE | 285 | 27.157 | 89.301 | 10.171 | 1.00 | 15.00 | A |
| | ATOM | 1352 | CD1 | ILE | 285 | 25.781 | 89.470 | 9.533 | 1.00 | 16.25 | A |
| 35 | ATOM | 1353 | C | ILE | 285 | 28.427 | 87.958 | 13.618 | 1.00 | 18.61 | A |
| | ATOM | 1354 | O | ILE | 285 | 27.631 | 87.083 | 13.985 | 1.00 | 20.11 | A |
| | ATOM | 1355 | N | LEU | 286 | 29.295 | 88.521 | 14.465 | 1.00 | 17.38 | A |
| | ATOM | 1356 | H | LEU | 286 | 29.905 | 89.212 | 14.134 | 1.00 | 0.00 | A |
| | ATOM | 1357 | CA | LEU | 286 | 29.348 | 88.131 | 15.884 | 1.00 | 17.79 | A |
| 40 | ATOM | 1358 | CB | LEU | 286 | 30.798 | 88.163 | 16.409 | 1.00 | 20.85 | A |
| | ATOM | 1359 | CG | LEU | 286 | 31.846 | 87.099 | 16.069 | 1.00 | 23.26 | A |
| | ATOM | 1360 | CD1 | LEU | 286 | 32.975 | 87.139 | 17.093 | 1.00 | 26.78 | A |
| | ATOM | 1361 | CD2 | LEU | 286 | 31.217 | 85.739 | 16.067 | 1.00 | 25.33 | A |
| | ATOM | 1362 | C | LEU | 286 | 28.501 | 89.056 | 16.754 | 1.00 | 18.17 | A |
| 45 | ATOM | 1363 | O | LEU | 286 | 28.515 | 88.951 | 17.983 | 1.00 | 20.22 | A |
| | ATOM | 1364 | N | GLY | 287 | 27.788 | 89.969 | 16.099 | 1.00 | 22.67 | A |
| | ATOM | 1365 | H | GLY | 287 | 27.840 | 89.999 | 15.120 | 1.00 | 0.00 | A |
| | ATOM | 1366 | CA | GLY | 287 | 26.941 | 90.925 | 16.789 | 1.00 | 20.22 | A |
| | ATOM | 1367 | C | GLY | 287 | 26.080 | 90.382 | 17.913 | 1.00 | 16.26 | A |
| 50 | ATOM | 1368 | O | GLY | 287 | 26.381 | 90.585 | 19.089 | 1.00 | 23.96 | A |
| | ATOM | 1369 | N | HIS | 288 | 25.000 | 89.693 | 17.572 | 1.00 | 22.56 | A |
| | ATOM | 1370 | H | HIS | 288 | 24.798 | 89.534 | 16.627 | 1.00 | 0.00 | A |
| | ATOM | 1371 | CA | HIS | 288 | 24.109 | 89.168 | 18.608 | 1.00 | 20.44 | A |
| | ATOM | 1372 | CB | HIS | 288 | 22.990 | 88.312 | 17.970 | 1.00 | 19.88 | A |
| 55 | ATOM | 1373 | CG | HIS | 288 | 21.974 | 87.804 | 18.950 | 1.00 | 23.39 | A |
| | ATOM | 1374 | CD2 | HIS | 288 | 21.917 | 86.650 | 19.654 | 1.00 | 17.27 | A |
| | ATOM | 1375 | ND1 | HIS | 288 | 20.917 | 88.571 | 19.385 | 1.00 | 15.20 | A |
| | ATOM | 1376 | HD1 | HIS | 288 | 20.679 | 89.455 | 19.045 | 1.00 | 0.00 | A |
| | ATOM | 1377 | CE1 | HIS | 288 | 20.242 | 87.909 | 20.310 | 1.00 | 15.13 | A |
| 60 | ATOM | 1378 | NE2 | HIS | 288 | 20.832 | 86.739 | 20.494 | 1.00 | 13.24 | A |
| | ATOM | 1379 | HE2 | HIS | 288 | 20.535 | 86.056 | 21.118 | 1.00 | 0.00 | A |
| | ATOM | 1380 | C | HIS | 288 | 24.850 | 88.371 | 19.715 | 1.00 | 17.46 | A |
| | ATOM | 1381 | O | HIS | 288 | 24.579 | 88.541 | 20.902 | 1.00 | 17.25 | A |
| | ATOM | 1382 | N | TYR | 289 | 25.798 | 87.525 | 19.334 | 1.00 | 18.14 | A |
| 65 | ATOM | 1383 | H | TYR | 289 | 26.023 | 87.431 | 18.384 | 1.00 | 0.00 | A |
| | ATOM | 1384 | CA | TYR | 289 | 26.505 | 86.737 | 20.330 | 1.00 | 16.63 | A |
| | ATOM | 1385 | CB | TYR | 289 | 27.405 | 85.709 | 19.647 | 1.00 | 25.01 | A |
| | ATOM | 1386 | CG | TYR | 289 | 26.727 | 84.387 | 19.312 | 1.00 | 26.14 | A |
| | ATOM | 1387 | CD1 | TYR | 289 | 25.631 | 84.330 | 18.449 | 1.00 | 26.68 | A |
| 70 | ATOM | 1388 | CE1 | TYR | 289 | 25.073 | 83.092 | 18.064 | 1.00 | 29.84 | A |
| | ATOM | 1389 | CD2 | TYR | 289 | 27.245 | 83.176 | 19.792 | 1.00 | 29.68 | A |
| | ATOM | 1390 | CE2 | TYR | 289 | 26.697 | 81.941 | 19.415 | 1.00 | 19.88 | A |
| | ATOM | 1391 | CZ | TYR | 289 | 25.624 | 81.904 | 18.551 | 1.00 | 24.45 | A |
| | ATOM | 1392 | OH | TYR | 289 | 25.129 | 80.680 | 18.154 | 1.00 | 29.76 | A |
| | ATOM | 1393 | HH | TYR | 289 | 24.390 | 80.813 | 17.553 | 1.00 | 0.00 | A |
| | ATOM | 1394 | C | TYR | 289 | 27.323 | 87.613 | 21.277 | 1.00 | 20.22 | A |
| | ATOM | 1395 | O | TYR | 289 | 27.369 | 87.356 | 22.481 | 1.00 | 19.02 | A |

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|----|------|------|------|-----|-----|--------|--------|----------|------|-------|---|
| 5 | ATOM | 1396 | N | ASN | 290 | 27.956 | 88.655 | 20.750 | 1.00 | 18.81 | A |
| | ATOM | 1397 | H | ASN | 290 | 27.904 | 88.835 | 19.789 | 1.00 | 0.00 | A |
| | ATOM | 1398 | CA | ASN | 290 | 28.739 | 89.532 | 21.621 | 1.00 | 15.76 | A |
| | ATOM | 1399 | CB | ASN | 290 | 29.625 | 90.469 | 20.804 | 1.00 | 19.19 | A |
| | ATOM | 1400 | CG | ASN | 290 | 30.840 | 89.780 | 20.231 | 1.00 | 22.46 | A |
| 10 | ATOM | 1401 | OD1 | ASN | 290 | 31.270 | 88.736 | 20.715 | 1.00 | 23.52 | A |
| | ATOM | 1402 | ND2 | ASN | 290 | 31.400 | 90.370 | 19.186 | 1.00 | 25.92 | A |
| | ATOM | 1403 | HD21 | ASN | 290 | 31.020 | 91.202 | 18.832 | 1.00 | 0.00 | A |
| | ATOM | 1404 | HD22 | ASN | 290 | 32.188 | 89.942 | 18.796 | 1.00 | 0.00 | A |
| | ATOM | 1405 | C | ASN | 290 | 27.822 | 90.378 | 22.493 | 1.00 | 15.64 | A |
| 15 | ATOM | 1406 | O | ASN | 290 | 28.108 | 90.600 | 23.672 | 1.00 | 23.61 | A |
| | ATOM | 1407 | N | ARG | 291 | 26.723 | 90.865 | 21.924 | 1.00 | 15.28 | A |
| | ATOM | 1408 | H | ARG | 291 | 26.524 | 90.672 | 20.984 | 1.00 | 0.00 | A |
| | ATOM | 1409 | CA | ARG | 291 | 25.812 | 91.687 | 22.713 | 1.00 | 14.06 | A |
| | ATOM | 1410 | CB | ARG | 291 | 24.679 | 92.252 | 21.845 | 1.00 | 16.24 | A |
| 20 | ATOM | 1411 | CG | ARG | 291 | 25.183 | 93.144 | 20.702 | 1.00 | 24.29 | A |
| | ATOM | 1412 | CD | ARG | 291 | 24.091 | 94.025 | 20.084 | 1.00 | 29.20 | A |
| | ATOM | 1413 | NE | ARG | 291 | 23.283 | 93.333 | 19.077 | 1.00 | 19.59 | A |
| | ATOM | 1414 | HE | ARG | 291 | 22.365 | 93.092 | 19.317 | 1.00 | 0.00 | A |
| | ATOM | 1415 | CZ | ARG | 291 | 23.709 | 93.013 | 17.859 | 1.00 | 34.23 | A |
| 25 | ATOM | 1416 | NH1 | ARG | 291 | 24.948 | 93.323 | 17.484 | 1.00 | 34.45 | A |
| | ATOM | 1417 | HH11 | ARG | 291 | 25.559 | 93.796 | 18.117 | 1.00 | 0.00 | A |
| | ATOM | 1418 | HH12 | ARG | 291 | 25.268 | 93.078 | 16.568 | 1.00 | 0.00 | A |
| | ATOM | 1419 | NH2 | ARG | 291 | 22.898 | 92.381 | 17.014 | 1.00 | 30.49 | A |
| | ATOM | 1420 | HH21 | ARG | 291 | 21.967 | 92.149 | 17.292 | 1.00 | 0.00 | A |
| 30 | ATOM | 1421 | HH22 | ARG | 291 | 23.222 | 92.139 | 16.099 | 1.00 | 0.00 | A |
| | ATOM | 1422 | C | ARG | 291 | 25.268 | 90.835 | 23.845 | 1.00 | 12.25 | A |
| | ATOM | 1423 | O | ARG | 291 | 25.073 | 91.317 | 24.963 | 1.00 | 17.10 | A |
| | ATOM | 1424 | N | GLY | 292 | 25.073 | 89.551 | 23.576 | 1.00 | 13.55 | A |
| | ATOM | 1425 | H | GLY | 292 | 25.286 | 89.193 | 22.690 | 1.00 | 0.00 | A |
| 35 | ATOM | 1426 | CA | GLY | 292 | 24.534 | 88.675 | 24.616 | 1.00 | 11.54 | A |
| | ATOM | 1427 | C | GLY | 292 | 25.542 | 88.057 | 25.562 | 1.00 | 22.48 | A |
| | ATOM | 1428 | O | GLY | 292 | 25.169 | 87.246 | 26.411 | 1.00 | 30.06 | A |
| | ATOM | 1429 | N | ASN | 293 | 26.813 | 88.425 | 25.422 | 1.00 | 25.61 | A |
| | ATOM | 1430 | H | ASN | 293 | 27.049 | 89.065 | 24.719 | 1.00 | 0.00 | A |
| 40 | ATOM | 1431 | CA | ASN | 293 | 27.867 | 87.897 | 26.281 | 1.00 | 29.06 | A |
| | ATOM | 1432 | CB | ASN | 293 | 27.567 | 88.238 | 27.750 | 1.00 | 33.48 | A |
| | ATOM | 1433 | CG | ASN | 293 | 27.687 | 89.741 | 28.058 | 1.00 | 41.34 | A |
| | ATOM | 1434 | OD1 | ASN | 293 | 27.506 | 90.595 | 27.185 | 1.00 | 41.61 | A |
| | ATOM | 1435 | ND2 | ASN | 293 | 27.988 | 90.060 | 29.319 | 1.00 | 40.94 | A |
| 45 | ATOM | 1436 | HD21 | ASN | 293 | 28.120 | 89.353 | 29.985 | 1.00 | 0.00 | A |
| | ATOM | 1437 | HD22 | ASN | 293 | 28.069 | 91.011 | 29.537</ | | | |

| | | | | | | | | | | | |
|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|---|
| | ATOM | 1469 | CB | GLU | 297 | 35.065 | 79.416 | 21.036 | 1.00 | 45.48 | A |
| | ATOM | 1470 | CG | GLU | 297 | 34.108 | 79.377 | 22.233 | 1.00 | 56.35 | A |
| | ATOM | 1471 | CD | GLU | 297 | 32.848 | 78.554 | 21.977 | 1.00 | 58.88 | A |
| | ATOM | 1472 | OE1 | GLU | 297 | 32.842 | 77.338 | 22.267 | 1.00 | 60.54 | A |
| 5 | ATOM | 1473 | OE2 | GLU | 297 | 31.855 | 79.130 | 21.489 | 1.00 | 62.33 | A |
| | ATOM | 1474 | C | GLU | 297 | 34.086 | 79.024 | 18.772 | 1.00 | 35.45 | A |
| | ATOM | 1475 | O | GLU | 297 | 34.729 | 78.809 | 17.748 | 1.00 | 34.80 | A |
| | ATOM | 1476 | N | LYS | 298 | 32.982 | 78.356 | 19.074 | 1.00 | 34.37 | A |
| | ATOM | 1477 | H | LYS | 298 | 32.498 | 78.581 | 19.895 | 1.00 | 0.00 | A |
| 10 | ATOM | 1478 | CA | LYS | 298 | 32.466 | 77.300 | 18.213 | 1.00 | 35.58 | A |
| | ATOM | 1479 | CB | LYS | 298 | 31.520 | 76.414 | 19.007 | 1.00 | 31.26 | A |
| | ATOM | 1480 | CG | LYS | 298 | 32.038 | 75.026 | 19.221 | 1.00 | 41.82 | A |
| | ATOM | 1481 | CD | LYS | 298 | 30.941 | 74.125 | 19.729 | 1.00 | 42.14 | A |
| | ATOM | 1482 | CE | LYS | 298 | 31.135 | 73.832 | 21.200 | 1.00 | 46.89 | A |
| 15 | ATOM | 1483 | NZ | LYS | 298 | 32.466 | 74.301 | 21.688 | 1.00 | 50.64 | A |
| | ATOM | 1484 | HZ1 | LYS | 298 | 32.544 | 75.328 | 21.550 | 1.00 | 0.00 | A |
| | ATOM | 1485 | HZ2 | LYS | 298 | 33.219 | 73.820 | 21.158 | 1.00 | 0.00 | A |
| | ATOM | 1486 | HZ3 | LYS | 298 | 32.559 | 74.079 | 22.701 | 1.00 | 0.00 | A |
| | ATOM | 1487 | C | LYS | 298 | 31.743 | 77.850 | 16.992 | 1.00 | 31.74 | A |
| 20 | ATOM | 1488 | O | LYS | 298 | 31.765 | 77.236 | 15.922 | 1.00 | 32.24 | A |
| | ATOM | 1489 | N | PHE | 299 | 31.101 | 79.005 | 17.170 | 1.00 | 29.34 | A |
| | ATOM | 1490 | H | PHE | 299 | 31.131 | 79.425 | 18.053 | 1.00 | 0.00 | A |
| | ATOM | 1491 | CA | PHE | 299 | 30.353 | 79.673 | 16.102 | 1.00 | 28.31 | A |
| | ATOM | 1492 | CB | PHE | 299 | 29.612 | 80.883 | 16.703 | 1.00 | 27.71 | A |
| 25 | ATOM | 1493 | CG | PHE | 299 | 29.131 | 81.904 | 15.699 | 1.00 | 19.45 | A |
| | ATOM | 1494 | CD1 | PHE | 299 | 28.503 | 81.526 | 14.516 | 1.00 | 15.16 | A |
| | ATOM | 1495 | CD2 | PHE | 299 | 29.287 | 83.261 | 15.964 | 1.00 | 16.16 | A |
| | ATOM | 1496 | CE1 | PHE | 299 | 28.046 | 82.496 | 13.616 | 1.00 | 15.54 | A |
| | ATOM | 1497 | CE2 | PHE | 299 | 28.832 | 84.227 | 15.075 | 1.00 | 9.30 | A |
| 30 | ATOM | 1498 | CZ | PHE | 299 | 28.215 | 83.851 | 13.903 | 1.00 | 7.56 | A |
| | ATOM | 1499 | C | PHE | 299 | 31.296 | 80.076 | 14.966 | 1.00 | 27.62 | A |
| | ATOM | 1500 | O | PHE | 299 | 30.999 | 79.828 | 13.803 | 1.00 | 23.92 | A |
| | ATOM | 1501 | N | VAL | 300 | 32.440 | 80.667 | 15.300 | 1.00 | 32.50 | A |
| | ATOM | 1502 | H | VAL | 300 | 32.635 | 80.834 | 16.246 | 1.00 | 0.00 | A |
| 35 | ATOM | 1503 | CA | VAL | 300 | 33.419 | 81.074 | 14.280 | 1.00 | 40.70 | A |
| | ATOM | 1504 | CB | VAL | 300 | 34.545 | 81.950 | 14.877 | 1.00 | 45.83 | A |
| | ATOM | 1505 | CG1 | VAL | 300 | 35.734 | 81.084 | 15.280 | 1.00 | 49.69 | A |
| | ATOM | 1506 | CG2 | VAL | 300 | 34.988 | 82.975 | 13.860 | 1.00 | 49.35 | A |
| | ATOM | 1507 | C | VAL | 300 | 34.082 | 79.887 | 13.575 | 1.00 | 39.59 | A |
| 40 | ATOM | 1508 | O | VAL | 300 | 34.426 | 79.974 | 12.399 | 1.00 | 39.52 | A |
| | ATOM | 1509 | N | GLU | 301 | 34.274 | 78.791 | 14.302 | 1.00 | 38.31 | A |
| | ATOM | 1510 | H | GLU | 301 | 34.001 | 78.787 | 15.244 | 1.00 | 0.00 | A |
| | ATOM | 1511 | CA | GLU | 301 | 34.879 | 77.597 | 13.736 | 1.00 | 39.63 | A |
| | ATOM | 1512 | CB | GLU | 301 | 35.240 | 76.607 | 14.849 | 1.00 | 49.28 | A |
| 45 | ATOM | 1513 | CG | GLU | 301 | 36.060 | 75.406 | 14.388 | 1.00 | 51.49 | A |
| | ATOM | 1514 | CD | GLU | 301 | 35.928 | 74.221 | 15.328 | 1.00 | 57.74 | A |
| | ATOM | 1515 | OE1 | GLU | 301 | 34.879 | 73.542 | 15.283 | 1.00 | 60.72 | A |
| | ATOM | 1516 | OE2 | GLU | 301 | 36.867 | 73.968 | 16.114 | 1.00 | 58.47 | A |
| | ATOM | 1517 | C | GLU | 301 | 33.933 | 76.932 | 12.742 | 1.00 | 37.25 | A |
| 50 | ATOM | 1518 | O | GLU | 301 | 34.360 | 76.469 | 11.695 | 1.00 | 34.80 | A |
| | ATOM | 1519 | N | GLU | 302 | 32.647 | 76.880 | 13.061 | 1.00 | 29.99 | A |
| | ATOM | 1520 | H | GLU | 302 | 32.332 | 77.260 | 13.909 | 1.00 | 0.00 | A |
| | ATOM | 1521 | CA | GLU | 302 | 31.713 | 76.254 | 12.144 | 1.00 | 29.62 | A |
| | ATOM | 1522 | CB | GLU | 302 | 30.345 | 76.072 | 12.800 | 1.00 | 29.29 | A |
| 55 | ATOM | 1523 | CG | GLU | 302 | 29.188 | 76.118 | 11.813 | 1.00 | 30.24 | A |
| | ATOM | 1524 | CD | GLU | 302 | 27.839 | 76.218 | 12.489 | 1.00 | 26.05 | A |
| | ATOM | 1525 | OE1 | GLU | 302 | 27.674 | 75.643 | 13.581 | 1.00 | 24.89 | A |
| | ATOM | 1526 | OE2 | GLU | 302 | 26.940 | 76.870 | 11.925 | 1.00 | 30.75 | A |
| | ATOM | 1527 | C | GLU | 302 | 31.574 | 77.093 | 10.874 | 1.00 | 32.99 | A |
| 60 | ATOM | 1528 | O | GLU | 302 | 31.445 | 76.549 | 9.775 | 1.00 | 30.91 | A |
| | ATOM | 1529 | N | ILE | 303 | 31.615 | 78.416 | 11.014 | 1.00 | 31.38 | A |
| | ATOM | 1530 | H | ILE | 303 | 31.732 | 78.810 | 11.904 | 1.00 | 0.00 | A |
| | ATOM | 1531 | CA | ILE | 303 | 31.486 | 79.283 | 9.842 | 1.00 | 31.29 | A |
| | ATOM | 1532 | CB | ILE | 303 | 31.187 | 80.752 | 10.241 | 1.00 | 28.58 | A |
| 65 | ATOM | 1533 | CG2 | ILE | 303 | 30.822 | 81.554 | 9.009 | 1.00 | 23.48 | A |
| | ATOM | 1534 | CG1 | ILE | 303 | 30.043 | 80.800 | 11.264 | 1.00 | 26.97 | A |
| | ATOM | 1535 | CD1 | ILE | 303 | 28.805 | 80.026 | 10.852 | 1.00 | 24.95 | A |
| | ATOM | 1536 | C | ILE | 303 | 32.773 | 79.228 | 9.029 | 1.00 | 33.05 | A |
| | ATOM | 1537 | O | ILE | 303 | 32.744 | 79.181 | 7.796 | 1.00 | 35.02 | A |
| 70 | ATOM | 1538 | N | LYS | 304 | 33.903 | 79.248 | 9.724 | 1.00 | 30.79 | A |
| | ATOM | 1539 | H | LYS | 304 | 33.869 | 79.332 | 10.698 | 1.00 | 0.00 | A |
| | ATOM | 1540 | CA | LYS | 304 | 35.190 | 79.150 | 9.060 | 1.00 | 30.72 | A |
| | ATOM | 1541 | CB | LYS | 304 | 36.298 | 78.979 | 10.118 | 1.00 | 33.59 | A |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1542 | CG | LYS | 304 | 37.724 | 79.320 | 9.642 | 1.00 | 41.97 | A |
| | ATOM | 1543 | CD | LYS | 304 | 38.511 | 80.155 | 10.667 | 1.00 | 41.17 | A |
| | ATOM | 1544 | CE | LYS | 304 | 39.416 | 81.173 | 9.976 | 1.00 | 42.05 | A |
| | ATOM | 1545 | NZ | LYS | 304 | 40.815 | 80.691 | 9.824 | 1.00 | 41.08 | A |
| | ATOM | 1546 | HZ1 | LYS | 304 | 40.823 | 79.820 | 9.256 | 1.00 | 0.00 | A |
| 10 | ATOM | 1547 | HZ2 | LYS | 304 | 41.217 | 80.495 | 10.764 | 1.00 | 0.00 | A |
| | ATOM | 1548 | HZ3 | LYS | 304 | 41.384 | 81.421 | 9.350 | 1.00 | 0.00 | A |
| | ATOM | 1549 | C | LYS | 304 | 35.100 | 77.904 | 8.161 | 1.00 | 25.59 | A |
| | ATOM | 1550 | O | LYS | 304 | 35.395 | 77.951 | 6.969 | 1.00 | 33.47 | A |
| | ATOM | 1551 | N | SER | 305 | 34.661 | 76.800 | 8.767 | 1.00 | 26.69 | A |
| 15 | ATOM | 1552 | H | SER | 305 | 34.433 | 76.870 | 9.716 | 1.00 | 0.00 | A |
| | ATOM | 1553 | CA | SER | 305 | 34.498 | 75.489 | 8.125 | 1.00 | 22.76 | A |
| | ATOM | 1554 | CB | SER | 305 | 33.932 | 74.498 | 9.144 | 1.00 | 27.40 | A |
| | ATOM | 1555 | OG | SER | 305 | 32.539 | 74.298 | 8.939 | 1.00 | 24.13 | A |
| | ATOM | 1556 | HG | SER | 305 | 32.075 | 75.133 | 9.030 | 1.00 | 0.00 | A |
| 20 | ATOM | 1557 | C | SER | 305 | 33.635 | 75.403 | 6.860 | 1.00 | 24.66 | A |
| | ATOM | 1558 | O | SER | 305 | 33.536 | 74.340 | 6.239 | 1.00 | 27.99 | A |
| | ATOM | 1559 | N | ILE | 306 | 32.983 | 76.490 | 6.482 | 1.00 | 25.24 | A |
| | ATOM | 1560 | H | ILE | 306 | 33.058 | 77.317 | 7.005 | 1.00 | 0.00 | A |
| | ATOM | 1561 | CA | ILE | 306 | 32.154 | 76.453 | 5.294 | 1.00 | 20.72 | A |
| 25 | ATOM | 1562 | CB | ILE | 306 | 30.828 | 77.211 | 5.513 | 1.00 | 17.86 | A |
| | ATOM | 1563 | CG2 | ILE | 306 | 30.078 | 77.326 | 4.209 | 1.00 | 20.63 | A |
| | ATOM | 1564 | CG1 | ILE | 306 | 29.952 | 76.448 | 6.510 | 1.00 | 20.49 | A |
| | ATOM | 1565 | CD1 | ILE | 306 | 29.382 | 77.307 | 7.603 | 1.00 | 19.14 | A |
| | ATOM | 1566 | C | ILE | 306 | 32.908 | 77.098 | 4.156 | 1.00 | 16.50 | A |
| 30 | ATOM | 1567 | O | ILE | 306 | 32.689 | 76.783 | 2.994 | 1.00 | 19.41 | A |
| | ATOM | 1568 | N | ALA | 307 | 33.833 | 77.979 | 4.499 | 1.00 | 22.89 | A |
| | ATOM | 1569 | H | ALA | 307 | 34.019 | 78.150 | 5.446 | 1.00 | 0.00 | A |
| | ATOM | 1570 | CA | ALA | 307 | 34.576 | 78.686 | 3.480 | 1.00 | 24.83 | A |
| | ATOM | 1571 | CB | ALA | 307 | 35.383 | 79.794 | 4.123 | 1.00 | 30.01 | A |
| 35 | ATOM | 1572 | C | ALA | 307 | 35.476 | 77.766 | 2.665 | 1.00 | 23.99 | A |
| | ATOM | 1573 | O | ALA | 307 | 36.047 | 76.812 | 3.187 | 1.00 | 21.83 | A |
| | ATOM | 1574 | N | SER | 308 | 35.568 | 78.035 | 1.368 | 1.00 | 23.95 | A |
| | ATOM | 1575 | H | SER | 308 | 35.037 | 78.765 | 0.987 | 1.00 | 0.00 | A |
| | ATOM | 1576 | CA | SER | 308 | 36.445 | 77.252 | 0.511 | 1.00 | 29.22 | A |
| 40 | ATOM | 1577 | CB | SER | 308 | 36.343 | 77.740 | -0.937 | 1.00 | 21.79 | A |
| | ATOM | 1578 | OG | SER | 308 | 35.241 | 77.145 | -1.606 | 1.00 | 28.41 | A |
| | ATOM | 1579 | HG | SER | 308 | 34.430 | 77.376 | -1.149 | 1.00 | 0.00 | A |
| | ATOM | 1580 | C | SER | 308 | 37.870 | 77.489 | 1.035 | 1.00 | 34.88 | A |
| | ATOM | 1581 | O | SER | 308 | 38.119 | 78.483 | 1.724 | 1.00 | 32.75 | A |
| 45 | ATOM | 1582 | N | GLU | 309 | 38.795 | 76.581 | 0.722 | 1.00 | 40.30 | A |
| | ATOM | 1583 | H | GLU | 309 | 38.537 | 75.801 | 0.188 | 1.00 | 0.00 | A |
| | ATOM | 1584 | CA | GL | | | | | | | |

| | | | | | | | | | | | |
|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| | ATOM | 1615 | OE2 | GLU | 312 | 43.559 | 80.274 | 7.394 | 1.00 | 47.20 | A |
| | ATOM | 1616 | C | GLU | 312 | 41.502 | 83.747 | 4.724 | 1.00 | 41.45 | A |
| | ATOM | 1617 | O | GLU | 312 | 41.404 | 84.963 | 4.901 | 1.00 | 41.26 | A |
| 5 | ATOM | 1618 | N | LYS | 313 | 41.317 | 83.181 | 3.542 | 1.00 | 37.88 | A |
| | ATOM | 1619 | H | LYS | 313 | 41.394 | 82.207 | 3.451 | 1.00 | 0.00 | A |
| | ATOM | 1620 | CA | LYS | 313 | 40.997 | 83.993 | 2.380 | 1.00 | 36.21 | A |
| | ATOM | 1621 | CB | LYS | 313 | 41.564 | 83.358 | 1.116 | 1.00 | 33.23 | A |
| | ATOM | 1622 | CG | LYS | 313 | 41.563 | 84.300 | -0.079 | 1.00 | 34.65 | A |
| 10 | ATOM | 1623 | CD | LYS | 313 | 41.058 | 83.617 | -1.335 | 1.00 | 27.45 | A |
| | ATOM | 1624 | CE | LYS | 313 | 39.861 | 84.348 | -1.905 | 1.00 | 29.91 | A |
| | ATOM | 1625 | NZ | LYS | 313 | 39.913 | 84.435 | -3.387 | 1.00 | 32.98 | A |
| | ATOM | 1626 | HZ1 | LYS | 313 | 39.928 | 83.476 | -3.790 | 1.00 | 0.00 | A |
| | ATOM | 1627 | HZ2 | LYS | 313 | 40.770 | 84.946 | -3.674 | 1.00 | 0.00 | A |
| | ATOM | 1628 | HZ3 | LYS | 313 | 39.073 | 84.941 | -3.733 | 1.00 | 0.00 | A |
| 15 | ATOM | 1629 | C | LYS | 313 | 39.515 | 84.249 | 2.159 | 1.00 | 37.37 | A |
| | ATOM | 1630 | O | LYS | 313 | 39.132 | 85.357 | 1.789 | 1.00 | 40.91 | A |
| | ATOM | 1631 | N | HIS | 314 | 38.683 | 83.234 | 2.385 | 1.00 | 32.67 | A |
| | ATOM | 1632 | H | HIS | 314 | 39.036 | 82.382 | 2.718 | 1.00 | 0.00 | A |
| 20 | ATOM | 1633 | CA | HIS | 314 | 37.250 | 83.372 | 2.143 | 1.00 | 34.37 | A |
| | ATOM | 1634 | CB | HIS | 314 | 36.725 | 82.171 | 1.343 | 1.00 | 33.80 | A |
| | ATOM | 1635 | CG | HIS | 314 | 37.658 | 81.682 | 0.280 | 1.00 | 29.70 | A |
| | ATOM | 1636 | CD2 | HIS | 314 | 38.910 | 81.168 | 0.360 | 1.00 | 31.43 | A |
| | ATOM | 1637 | ND1 | HIS | 314 | 37.307 | 81.631 | -1.051 | 1.00 | 29.34 | A |
| | ATOM | 1638 | HD1 | HIS | 314 | 36.455 | 81.936 | -1.435 | 1.00 | 0.00 | A |
| 25 | ATOM | 1639 | CE1 | HIS | 314 | 38.295 | 81.109 | -1.747 | 1.00 | 29.33 | A |
| | ATOM | 1640 | NE2 | HIS | 314 | 39.283 | 80.818 | -0.914 | 1.00 | 29.14 | A |
| | ATOM | 1641 | HE2 | HIS | 314 | 40.137 | 80.421 | -1.175 | 1.00 | 0.00 | A |
| | ATOM | 1642 | C | HIS | 314 | 36.368 | 83.552 | 3.372 | 1.00 | 35.91 | A |
| 30 | ATOM | 1643 | O | HIS | 314 | 35.184 | 83.860 | 3.239 | 1.00 | 41.62 | A |
| | ATOM | 1644 | N | PHE | 315 | 36.920 | 83.340 | 4.559 | 1.00 | 36.72 | A |
| | ATOM | 1645 | H | PHE | 315 | 37.858 | 83.065 | 4.622 | 1.00 | 0.00 | A |
| | ATOM | 1646 | CA | PHE | 315 | 36.132 | 83.512 | 5.770 | 1.00 | 37.19 | A |
| | ATOM | 1647 | CB | PHE | 315 | 36.552 | 82.493 | 6.834 | 1.00 | 34.33 | A |
| 35 | ATOM | 1648 | CG | PHE | 315 | 36.038 | 82.804 | 8.214 | 1.00 | 26.72 | A |
| | ATOM | 1649 | CD1 | PHE | 315 | 34.684 | 82.672 | 8.519 | 1.00 | 30.96 | A |
| | ATOM | 1650 | CD2 | PHE | 315 | 36.911 | 83.225 | 9.213 | 1.00 | 25.93 | A |
| | ATOM | 1651 | CE1 | PHE | 315 | 34.209 | 82.955 | 9.800 | 1.00 | 23.91 | A |
| | ATOM | 1652 | CE2 | PHE | 315 | 36.451 | 83.510 | 10.494 | 1.00 | 28.16 | A |
| 40 | ATOM | 1653 | CZ | PHE | 315 | 35.094 | 83.375 | 10.788 | 1.00 | 29.32 | A |
| | ATOM | 1654 | C | PHE | 315 | 36.326 | 84.928 | 6.299 | 1.00 | 38.47 | A |
| | ATOM | 1655 | O | PHE | 315 | 37.449 | 85.428 | 6.344 | 1.00 | 41.30 | A |
| | ATOM | 1656 | N | PHE | 316 | 35.219 | 85.561 | 6.685 | 1.00 | 36.02 | A |
| | ATOM | 1657 | H | PHE | 316 | 34.364 | 85.091 | 6.602 | 1.00 | 0.00 | A |
| 45 | ATOM | 1658 | CA | PHE | 316 | 35.213 | 86.918 | 7.223 | 1.00 | 32.16 | A |
| | ATOM | 1659 | CB | PHE | 316 | 34.390 | 87.856 | 6.334 | 1.00 | 31.62 | A |
| | ATOM | 1660 | CG | PHE | 316 | 35.057 | 88.194 | 5.041 | 1.00 | 37.01 | A |
| | ATOM | 1661 | CD1 | PHE | 316 | 34.804 | 87.437 | 3.898 | 1.00 | 29.79 | A |
| | ATOM | 1662 | CD2 | PHE | 316 | 35.979 | 89.233 | 4.971 | 1.00 | 33.37 | A |
| 50 | ATOM | 1663 | CE1 | PHE | 316 | 35.462 | 87.705 | 2.713 | 1.00 | 33.51 | A |
| | ATOM | 1664 | CE2 | PHE | 316 | 36.644 | 89.511 | 3.786 | 1.00 | 37.63 | A |
| | ATOM | 1665 | CZ | PHE | 316 | 36.388 | 88.745 | 2.653 | 1.00 | 37.22 | A |
| | ATOM | 1666 | C | PHE | 316 | 34.577 | 86.895 | 8.596 | 1.00 | 30.46 | A |
| | ATOM | 1667 | O | PHE | 316 | 33.446 | 86.467 | 8.751 | 1.00 | 28.70 | A |
| 55 | ATOM | 1668 | N | ASN | 317 | 35.311 | 87.355 | 9.591 | 1.00 | 30.17 | A |
| | ATOM | 1669 | H | ASN | 317 | 36.220 | 87.668 | 9.414 | 1.00 | 0.00 | A |
| | ATOM | 1670 | CA | ASN | 317 | 34.795 | 87.405 | 10.939 | 1.00 | 31.72 | A |
| | ATOM | 1671 | CB | ASN | 317 | 35.855 | 86.917 | 11.927 | 1.00 | 29.33 | A |
| | ATOM | 1672 | CG | ASN | 317 | 35.485 | 87.205 | 13.376 | 1.00 | 34.11 | A |
| 60 | ATOM | 1673 | OD1 | ASN | 317 | 34.771 | 88.163 | 13.667 | 1.00 | 38.43 | A |
| | ATOM | 1674 | ND2 | ASN | 317 | 35.983 | 86.375 | 14.289 | 1.00 | 32.35 | A |
| | ATOM | 1675 | HD21 | ASN | 317 | 36.553 | 85.627 | 14.018 | 1.00 | 0.00 | A |
| | ATOM | 1676 | HD22 | ASN | 317 | 35.752 | 86.550 | 15.226 | 1.00 | 0.00 | A |
| | ATOM | 1677 | C | ASN | 317 | 34.442 | 88.861 | 11.197 | 1.00 | 33.41 | A |
| 65 | ATOM | 1678 | O | ASN | 317 | 35.325 | 89.686 | 11.440 | 1.00 | 35.10 | A |
| | ATOM | 1679 | N | VAL | 318 | 33.152 | 89.175 | 11.128 | 1.00 | 34.27 | A |
| | ATOM | 1680 | H | VAL | 318 | 32.498 | 88.478 | 10.922 | 1.00 | 0.00 | A |
| | ATOM | 1681 | CA | VAL | 318 | 32.689 | 90.543 | 11.355 | 1.00 | 32.08 | A |
| | ATOM | 1682 | CB | VAL | 318 | 31.629 | 90.958 | 10.301 | 1.00 | 36.04 | A |
| 70 | ATOM | 1683 | CG1 | VAL | 318 | 31.316 | 92.441 | 10.426 | 1.00 | 35.17 | A |
| | ATOM | 1684 | CG2 | VAL | 318 | 32.147 | 90.660 | 8.905 | 1.00 | 37.95 | A |
| | ATOM | 1685 | C | VAL | 318 | 32.123 | 90.743 | 12.762 | 1.00 | 25.89 | A |
| | ATOM | 1686 | O | VAL | 318 | 31.293 | 89.978 | 13.238 | 1.00 | 27.33 | A |
| | ATOM | 1687 | N | SER | 319 | 32.618 | 91.790 | 13.406 | 1.00 | 23.18 | A |

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|----|------|------|-----|-----|-----|--------|---------|--------|------|-------|---|
| 5 | ATOM | 1688 | H | SER | 319 | 33.278 | 92.338 | 12.932 | 1.00 | 0.00 | A |
| | ATOM | 1689 | CA | SER | 319 | 32.261 | 92.198 | 14.757 | 1.00 | 22.35 | A |
| | ATOM | 1690 | CB | SER | 319 | 32.972 | 93.523 | 15.071 | 1.00 | 21.96 | A |
| | ATOM | 1691 | OG | SER | 319 | 33.554 | 93.517 | 16.360 | 1.00 | 35.71 | A |
| | ATOM | 1692 | HG | SER | 319 | 34.201 | 92.809 | 16.416 | 1.00 | 0.00 | A |
| 10 | ATOM | 1693 | C | SER | 319 | 30.765 | 92.371 | 14.988 | 1.00 | 22.88 | A |
| | ATOM | 1694 | O | SER | 319 | 30.212 | 91.854 | 15.959 | 1.00 | 20.95 | A |
| | ATOM | 1695 | N | ASP | 320 | 30.128 | 93.157 | 14.125 | 1.00 | 25.15 | A |
| | ATOM | 1696 | H | ASP | 320 | 30.632 | 93.579 | 13.399 | 1.00 | 0.00 | A |
| | ATOM | 1697 | CA | ASP | 320 | 28.698 | 93.400 | 14.232 | 1.00 | 23.64 | A |
| 15 | ATOM | 1698 | CB | ASP | 320 | 28.383 | 94.447 | 15.334 | 1.00 | 30.33 | A |
| | ATOM | 1699 | CG | ASP | 320 | 29.128 | 95.762 | 15.156 | 1.00 | 27.91 | A |
| | ATOM | 1700 | OD1 | ASP | 320 | 30.369 | 95.774 | 15.088 | 1.00 | 27.84 | A |
| | ATOM | 1701 | OD2 | ASP | 320 | 28.456 | 96.799 | 15.098 | 1.00 | 30.37 | A |
| | ATOM | 1702 | C | ASP | 320 | 28.093 | 93.791 | 12.896 | 1.00 | 21.79 | A |
| 20 | ATOM | 1703 | O | ASP | 320 | 28.796 | 93.896 | 11.893 | 1.00 | 21.85 | A |
| | ATOM | 1704 | N | GLU | 321 | 26.781 | 93.982 | 12.878 | 1.00 | 23.98 | A |
| | ATOM | 1705 | H | GLU | 321 | 26.274 | 93.890 | 13.711 | 1.00 | 0.00 | A |
| | ATOM | 1706 | CA | GLU | 321 | 26.077 | 94.326 | 11.652 | 1.00 | 25.27 | A |
| | ATOM | 1707 | CB | GLU | 321 | 24.565 | 94.361 | 11.920 | 1.00 | 24.89 | A |
| 25 | ATOM | 1708 | CG | GLU | 321 | 23.954 | 92.980 | 12.285 | 1.00 | 16.77 | A |
| | ATOM | 1709 | CD | GLU | 321 | 23.945 | 92.711 | 13.793 | 1.00 | 16.37 | A |
| | ATOM | 1710 | OE1 | GLU | 321 | 24.672 | 93.402 | 14.533 | 1.00 | 17.10 | A |
| | ATOM | 1711 | OE2 | GLU | 321 | 23.203 | 91.815 | 14.244 | 1.00 | 21.60 | A |
| | ATOM | 1712 | C | GLU | 321 | 26.547 | 95.638 | 11.019 | 1.00 | 30.46 | A |
| 30 | ATOM | 1713 | O | GLU | 321 | 26.682 | 95.733 | 9.795 | 1.00 | 26.52 | A |
| | ATOM | 1714 | N | LEU | 322 | 26.804 | 96.649 | 11.847 | 1.00 | 30.02 | A |
| | ATOM | 1715 | H | LEU | 322 | 26.680 | 96.524 | 12.809 | 1.00 | 0.00 | A |
| | ATOM | 1716 | CA | LEU | 322 | 27.266 | 97.937 | 11.338 | 1.00 | 33.52 | A |
| | ATOM | 1717 | CB | LEU | 322 | 27.371 | 98.959 | 12.480 | 1.00 | 24.65 | A |
| 35 | ATOM | 1718 | CG | LEU | 322 | 26.103 | 99.774 | 12.671 | 1.00 | 21.95 | A |
| | ATOM | 1719 | CD1 | LEU | 322 | 26.344 | 100.939 | 13.616 | 1.00 | 25.01 | A |
| | ATOM | 1720 | CD2 | LEU | 322 | 25.653 | 100.267 | 11.323 | 1.00 | 29.24 | A |
| | ATOM | 1721 | C | LEU | 322 | 28.620 | 97.824 | 10.632 | 1.00 | 34.43 | A |
| | ATOM | 1722 | O | LEU | 322 | 28.860 | 98.497 | 9.630 | 1.00 | 38.95 | A |
| 40 | ATOM | 1723 | N | ALA | 323 | 29.492 | 96.962 | 11.142 | 1.00 | 35.14 | A |
| | ATOM | 1724 | H | ALA | 323 | 29.236 | 96.426 | 11.923 | 1.00 | 0.00 | A |
| | ATOM | 1725 | CA | ALA | 323 | 30.826 | 96.790 | 10.569 | 1.00 | 35.03 | A |
| | ATOM | 1726 | CB | ALA | 323 | 31.768 | 96.217 | 11.625 | 1.00 | 35.40 | A |
| | ATOM | 1727 | C | ALA | 323 | 30.880 | 95.925 | 9.311 | 1.00 | 35.38 | A |
| 45 | ATOM | 1728 | O | ALA | 323 | 31.967 | 95.531 | 8.878 | 1.00 | 34.45 | A |
| | ATOM | 1729 | N | LEU | 324 | 29.718 | 95.632 | 8.730 | 1.00 | 33.27 | A |
| | ATOM | 1730 | H | LEU | 324 | 28.891 | 95.981 | 9.121 | 1.00 | 0.00 | A |
| | ATOM | 1731 | CA | LEU | 324 | 29.638 | 94.805 | 7.525 | 1.00 | 30.65 | A |
| | ATOM | 1732 | CB | LEU | 324 | 28.199 | 94.313 | 7.308 | 1.00 | 28.08 | A |
| 50 | ATOM | 1733 | CG | LEU | 324 | 27.672 | 92.979 | 7.874 | 1.00 | 27.13 | A |
| | ATOM | 1734 | CD1 | LEU | 324 | 26.168 | 92.949 | 7.666 | 1.00 | 24.21 | A |
| | ATOM | 1735 | CD2 | LEU | 324 | 28.304 | 91.773 | 7.178 | 1.00 | 24.75 | A |
| | ATOM | 1736 | C | LEU | 324 | 30.086 | 95.604 | 6.296 | 1.00 | 37.04 | A |
| | ATOM | 1737 | O | LEU | 324 | 30.858 | 95.116 | 5.471 | 1.00 | 31.90 | A |
| 55 | ATOM | 1738 | N | VAL | 325 | 29.601 | 96.841 | 6.193 | 1.00 | 40.73 | A |
| | ATOM | 1739 | H | VAL | 325 | 29.010 | 97.174 | 6.898 | 1.00 | 0.00 | A |
| | ATOM | 1740 | CA | VAL | 325 | 29.923 | 97.711 | 5.069 | 1.00 | 43.41 | A |
| | ATOM | 1741 | CB | VAL | 325 | 29.063 | 98.996 | 5.093 | 1.00 | 46.34 | A |
| | ATOM | 1742 | CG1 | VAL | 325 | 27.959 | 98.896 | 4.052 | 1.00 | 47.62 | A |
| 60 | ATOM | 1743 | CG2 | VAL | 325 | 28.470 | 99.209 | 6.474 | 1.00 | 51.12 | A |
| | ATOM | 1744 | C | VAL | 325 | 31.395 | 98.107 | 4.985 | 1.00 | 46.86 | A |
| | ATOM | 1745 | O | VAL | 325 | 31.759 | 99.028 | 4.248 | 1.00 | 48.27 | A |
| | ATOM | 1746 | N | THR | 326 | 32.241 | 97.409 | 5.736 | 1.00 | 45.92 | A |
| | ATOM | 1747 | H | THR | 326 | 31.892 | 96.697 | 6.310 | 1.00 | 0.00 | A |
| 65 | ATOM | 1748 | CA | THR | 326 | 33.672 | 97.677 | 5.729 | 1.00 | 48.06 | A |
| | ATOM | 1749 | CB | THR | 326 | 34.180 | 98.101 | 7.125 | 1.00 | 49.74 | A |
| | ATOM | 1750 | OG1 | THR | 326 | 34.656 | 96.949 | 7.830 | 1.00 | 53.08 | A |
| | ATOM | 1751 | HG1 | THR | 326 | 33.943 | 96.315 | 7.928 | 1.00 | 0.00 | A |
| | ATOM | 1752 | CG2 | THR | 326 | 33.063 | 98.756 | 7.926 | 1.00 | 52.68 | A |
| 70 | ATOM | 1753 | C | THR | 326 | 34.411 | 96.415 | 5.313 | 1.00 | 47.66 | A |
| | ATOM | 1754 | O | THR | 326 | 35.615 | 96.290 | 5.523 | 1.00 | 45.71 | A |
| | ATOM | 1755 | N | ILE | 327 | 33.675 | 95.479 | 4.725 | 1.00 | 50.08 | A |
| | ATOM | 1756 | H | ILE | 327 | 32.720 | 95.648 | 4.586 | 1.00 | 0.00 | A |
| | ATOM | 1757 | CA | ILE | 327 | 34.239 | 94.211 | 4.278 | 1.00 | 49.17 | A |
| | ATOM | 1758 | CB | ILE | 327 | 33.653 | 93.029 | 5.118 | 1.00 | 46.23 | A |
| | ATOM | 1759 | CG2 | ILE | 327 | 32.917 | 92.026 | 4.237 | 1.00 | 47.06 | A |
| | ATOM | 1760 | CG1 | ILE | 327 | 34.779 | 92.352 | 5.895 | 1.00 | 47.16 | A |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1761 | CD1 | ILE | 327 | 34.325 | 91.201 | 6.768 | 1.00 | 44.14 | A |
| | ATOM | 1762 | C | ILE | 327 | 33.936 | 94.026 | 2.793 | 1.00 | 50.56 | A |
| | ATOM | 1763 | O | ILE | 327 | 34.327 | 93.026 | 2.179 | 1.00 | 50.93 | A |
| | ATOM | 1764 | N | VAL | 328 | 33.261 | 95.020 | 2.220 | 1.00 | 49.92 | A |
| | ATOM | 1765 | H | VAL | 328 | 33.014 | 95.796 | 2.765 | 1.00 | 0.00 | A |
| 10 | ATOM | 1766 | CA | VAL | 328 | 32.878 | 94.998 | 0.812 | 1.00 | 53.12 | A |
| | ATOM | 1767 | CB | VAL | 328 | 31.947 | 96.172 | 0.479 | 1.00 | 51.75 | A |
| | ATOM | 1768 | CG1 | VAL | 328 | 30.573 | 95.931 | 1.085 | 1.00 | 53.91 | A |
| | ATOM | 1769 | CG2 | VAL | 328 | 32.552 | 97.465 | 1.000 | 1.00 | 52.78 | A |
| | ATOM | 1770 | C | VAL | 328 | 34.045 | 95.043 | -0.173 | 1.00 | 54.61 | A |
| 15 | ATOM | 1771 | O | VAL | 328 | 33.974 | 94.456 | -1.252 | 1.00 | 53.08 | A |
| | ATOM | 1772 | N | LYS | 329 | 35.114 | 95.745 | 0.190 | 1.00 | 56.00 | A |
| | ATOM | 1773 | H | LYS | 329 | 35.130 | 96.192 | 1.061 | 1.00 | 0.00 | A |
| | ATOM | 1774 | CA | LYS | 329 | 36.262 | 95.855 | -0.699 | 1.00 | 54.78 | A |
| | ATOM | 1775 | CB | LYS | 329 | 37.185 | 96.987 | -0.239 | 1.00 | 59.48 | A |
| 20 | ATOM | 1776 | CG | LYS | 329 | 37.135 | 98.218 | -1.130 | 1.00 | 62.07 | A |
| | ATOM | 1777 | CD | LYS | 329 | 35.950 | 99.103 | -0.777 | 1.00 | 64.89 | A |
| | ATOM | 1778 | CE | LYS | 329 | 34.651 | 98.580 | -1.372 | 1.00 | 68.36 | A |
| | ATOM | 1779 | NZ | LYS | 329 | 34.865 | 97.635 | -2.509 | 1.00 | 71.98 | A |
| | ATOM | 1780 | HZ1 | LYS | 329 | 35.410 | 96.815 | -2.184 | 1.00 | 0.00 | A |
| 25 | ATOM | 1781 | HZ2 | LYS | 329 | 35.385 | 98.117 | -3.268 | 1.00 | 0.00 | A |
| | ATOM | 1782 | HZ3 | LYS | 329 | 33.943 | 97.314 | -2.871 | 1.00 | 0.00 | A |
| | ATOM | 1783 | C | LYS | 329 | 37.053 | 94.565 | -0.841 | 1.00 | 51.87 | A |
| | ATOM | 1784 | O | LYS | 329 | 37.406 | 94.173 | -1.954 | 1.00 | 52.46 | A |
| | ATOM | 1785 | N | ALA | 330 | 37.320 | 93.902 | 0.280 | 1.00 | 47.32 | A |
| 30 | ATOM | 1786 | H | ALA | 330 | 36.995 | 94.257 | 1.134 | 1.00 | 0.00 | A |
| | ATOM | 1787 | CA | ALA | 330 | 38.085 | 92.663 | 0.264 | 1.00 | 46.18 | A |
| | ATOM | 1788 | CB | ALA | 330 | 38.581 | 92.348 | 1.659 | 1.00 | 42.75 | A |
| | ATOM | 1789 | C | ALA | 330 | 37.299 | 91.476 | -0.287 | 1.00 | 47.64 | A |
| | ATOM | 1790 | O | ALA | 330 | 37.877 | 90.567 | -0.876 | 1.00 | 47.07 | A |
| 35 | ATOM | 1791 | N | LEU | 331 | 35.984 | 91.484 | -0.089 | 1.00 | 49.91 | A |
| | ATOM | 1792 | H | LEU | 331 | 35.578 | 92.237 | 0.390 | 1.00 | 0.00 | A |
| | ATOM | 1793 | CA | LEU | 331 | 35.125 | 90.398 | -0.568 | 1.00 | 46.71 | A |
| | ATOM | 1794 | CB | LEU | 331 | 33.767 | 90.437 | 0.145 | 1.00 | 41.67 | A |
| | ATOM | 1795 | CG | LEU | 331 | 32.981 | 89.151 | 0.428 | 1.00 | 37.35 | A |
| 40 | ATOM | 1796 | CD1 | LEU | 331 | 31.508 | 89.445 | 0.260 | 1.00 | 38.69 | A |
| | ATOM | 1797 | CD2 | LEU | 331 | 33.395 | 88.028 | -0.493 | 1.00 | 32.33 | A |
| | ATOM | 1798 | C | LEU | 331 | 34.906 | 90.563 | -2.060 | 1.00 | 46.57 | A |
| | ATOM | 1799 | O | LEU | 331 | 34.938 | 89.595 | -2.817 | 1.00 | 44.39 | A |
| | ATOM | 1800 | N | GLY | 332 | 34.683 | 91.808 | -2.462 | 1.00 | 47.56 | A |
| 45 | ATOM | 1801 | H | GLY | 332 | 34.682 | 92.530 | -1.800 | 1.00 | 0.00 | A |
| | ATOM | 1802 | CA | GLY | 332 | 34.443 | 92.127 | -3.853 | 1.00 | 48.35 | A |
| | ATOM | 1803 | C | GLY | 332 | 35.651 | 91.998 | -4.753 | 1.00 | 49.41 | A |
| | ATOM | 1804 | O | GLY | 332 | 35.512 | 92.028 | -5.974 | 1.00 | 54.37 | A |
| | ATOM | 1805 | N | GLU | 333 | 36.840 | 91.870 | -4.177 | 1.00 | 48.21 | A |
| 50 | ATOM | 1806 | H | GLU | 333 | 36.918 | 91.872 | -3.200 | 1.00 | 0.00 | A |
| | ATOM | 1807 | CA | GLU | 333 | 38.023 | 91.727 | -5.008 | 1.00 | 44.83 | A |
| | ATOM | 1808 | CB | GLU | 333 | 39.113 | 92.733 | -4.593 | 1.00 | 44.79 | A |
| | ATOM | 1809 | CG | GLU | 333 | 40.169 | 92.276 | -3.598 | 1.00 | 44.17 | A |
| | ATOM | 1810 | CD | GLU | 333 | 40.917 | 93.463 | -2.986 | 1.00 | 43.91 | A |
| 55 | ATOM | 1811 | OE1 | GLU | 333 | 41.368 | 93.370 | -1.825 | 1.00 | 47.51 | A |
| | ATOM | 1812 | OE2 | GLU | 333 | 41.048 | 94.499 | -3.668 | 1.00 | 36.94 | A |
| | ATOM | 1813 | C | GLU | 333 | 38.506 | 90.289 | -4.953 | 1.00 | 42.92 | A |
| | ATOM | 1814 | O | GLU | 333 | 38.945 | 89.735 | -5.965 | 1.00 | 41.97 | A |
| | ATOM | 1815 | N | ARG | 334 | 38.387 | 89.669 | -3.784 | 1.00 | 35.56 | A |
| 60 | ATOM | 1816 | H | ARG | 334 | 38.029 | 90.155 | -3.013 | 1.00 | 0.00 | A |
| | ATOM | 1817 | CA | ARG | 334 | 38.789 | 88.274 | -3.638 | 1.00 | 41.85 | A |
| | ATOM | 1818 | CB | ARG | 334 | 38.733 | 87.861 | -2.171 | 1.00 | 39.37 | A |
| | ATOM | 1819 | CG | ARG | 334 | 39.742 | 88.555 | -1.305 | 1.00 | 38.56 | A |
| | ATOM | 1820 | CD | ARG | 334 | 39.589 | 88.107 | 0.118 | 1.00 | 37.12 | A |
| 65 | ATOM | 1821 | NE | ARG | 334 | 40.288 | 88.994 | 1.029 | 1.00 | 29.46 | A |
| | ATOM | 1822 | HE | ARG | 334 | 40.713 | 89.795 | 0.661 | 1.00 | 0.00 | A |
| | ATOM | 1823 | CZ | ARG | 334 | 40.367 | 88.791 | 2.338 | 1.00 | 34.98 | A |
| | ATOM | 1824 | NH1 | ARG | 334 | 39.786 | 87.737 | 2.880 | 1.00 | 31.07 | A |
| | ATOM | 1825 | HH11 | ARG | 334 | 39.264 | 87.104 | 2.308 | 1.00 | 0.00 | A |
| 70 | ATOM | 1826 | HH12 | ARG | 334 | 39.849 | 87.584 | 3.865 | 1.00 | 0.00 | A |
| | ATOM | 1827 | NH2 | ARG | 334 | 41.043 | 89.634 | 3.103 | 1.00 | 45.11 | A |
| | ATOM | 1828 | HH21 | ARG | 334 | 41.486 | 90.433 | 2.698 | 1.00 | 0.00 | A |
| | ATOM | 1829 | HH22 | ARG | 334 | 41.109 | 89.471 | 4.088 | 1.00 | 0.00 | A |
| | ATOM | 1830 | C | ARG | 334 | 37.846 | 87.374 | -4.448 | 1.00 | 44.22 | A |
| | ATOM | 1831 | O | ARG | 334 | 38.181 | 86.231 | -4.788 | 1.00 | 40.32 | A |
| | ATOM | 1832 | N | ILE | 335 | 36.662 | 87.903 | -4.748 | 1.00 | 44.23 | A |
| | ATOM | 1833 | H | ILE | 335 | 36.458 | 88.813 | -4.452 | 1.00 | 0.00 | A |

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|----|------|------|------|-----|-----|--------|--------|---------|------|-------|---|
| | ATOM | 1834 | CA | ILE | 335 | 35.663 | 87.164 | -5.504 | 1.00 | 45.07 | A |
| | ATOM | 1835 | CB | ILE | 335 | 34.260 | 87.798 | -5.329 | 1.00 | 46.64 | A |
| | ATOM | 1836 | CG2 | ILE | 335 | 34.330 | 89.285 | -5.585 | 1.00 | 50.46 | A |
| 5 | ATOM | 1837 | CG1 | ILE | 335 | 33.254 | 87.149 | -6.283 | 1.00 | 50.93 | A |
| | ATOM | 1838 | CD1 | ILE | 335 | 33.110 | 85.645 | -6.114 | 1.00 | 53.73 | A |
| | ATOM | 1839 | C | ILE | 335 | 36.045 | 87.134 | -6.977 | 1.00 | 41.85 | A |
| | ATOM | 1840 | O | ILE | 335 | 36.246 | 86.070 | -7.547 | 1.00 | 44.44 | A |
| | ATOM | 1841 | N | PHE | 336 | 36.159 | 88.304 | -7.591 | 1.00 | 38.93 | A |
| 10 | ATOM | 1842 | H | PHE | 336 | 35.995 | 89.130 | -7.093 | 1.00 | 0.00 | A |
| | ATOM | 1843 | CA | PHE | 336 | 36.526 | 88.371 | -8.994 | 1.00 | 40.81 | A |
| | ATOM | 1844 | CB | PHE | 336 | 36.041 | 89.684 | -9.590 | 1.00 | 34.92 | A |
| | ATOM | 1845 | CG | PHE | 336 | 34.548 | 89.816 | -9.618 | 1.00 | 30.97 | A |
| | ATOM | 1846 | CD1 | PHE | 336 | 33.895 | 90.694 | -8.753 | 1.00 | 30.10 | A |
| | ATOM | 1847 | CD2 | PHE | 336 | 33.792 | 89.072 | -10.513 | 1.00 | 29.08 | A |
| 15 | ATOM | 1848 | CE1 | PHE | 336 | 32.513 | 90.821 | -8.783 | 1.00 | 15.73 | A |
| | ATOM | 1849 | CE2 | PHE | 336 | 32.409 | 89.197 | -10.548 | 1.00 | 19.75 | A |
| | ATOM | 1850 | CZ | PHE | 336 | 31.772 | 90.078 | -9.677 | 1.00 | 20.19 | A |
| | ATOM | 1851 | C | PHE | 336 | 38.035 | 88.240 | -9.188 | 1.00 | 41.18 | A |
| 20 | ATOM | 1852 | O | PHE | 336 | 38.463 | 88.145 | -10.356 | 1.00 | 41.37 | A |
| | ATOM | 1853 | OT | PHE | 336 | 38.771 | 88.233 | -8.178 | 1.00 | 40.25 | A |
| | ATOM | 1854 | CB | ALA | 145 | 27.124 | 80.130 | 34.005 | 1.00 | 39.54 | B |
| | ATOM | 1855 | C | ALA | 145 | 25.323 | 81.127 | 32.585 | 1.00 | 38.62 | B |
| | ATOM | 1856 | O | ALA | 145 | 24.364 | 80.726 | 33.254 | 1.00 | 37.41 | B |
| 25 | ATOM | 1857 | HT1 | ALA | 145 | 26.147 | 82.508 | 34.837 | 1.00 | 0.00 | B |
| | ATOM | 1858 | HT2 | ALA | 145 | 26.612 | 83.408 | 33.474 | 1.00 | 0.00 | B |
| | ATOM | 1859 | N | ALA | 145 | 26.822 | 82.567 | 34.050 | 1.00 | 42.77 | B |
| | ATOM | 1860 | HT3 | ALA | 145 | 27.790 | 82.642 | 34.428 | 1.00 | 0.00 | B |
| | ATOM | 1861 | CA | ALA | 145 | 26.715 | 81.343 | 33.203 | 1.00 | 39.62 | B |
| 30 | ATOM | 1862 | N | GLN | 146 | 25.236 | 81.388 | 31.288 | 1.00 | 33.32 | B |
| | ATOM | 1863 | H | GLN | 146 | 26.034 | 81.700 | 30.819 | 1.00 | 0.00 | B |
| | ATOM | 1864 | CA | GLN | 146 | 24.004 | 81.230 | 30.537 | 1.00 | 31.87 | B |
| | ATOM | 1865 | CB | GLN | 146 | 24.024 | 82.162 | 29.354 | 1.00 | 29.22 | B |
| | ATOM | 1866 | CG | GLN | 146 | 23.274 | 83.421 | 29.543 | 1.00 | 34.86 | B |
| 35 | ATOM | 1867 | CD | GLN | 146 | 23.349 | 84.236 | 28.288 | 1.00 | 39.34 | B |
| | ATOM | 1868 | OE1 | GLN | 146 | 24.442 | 84.554 | 27.821 | 1.00 | 41.32 | B |
| | ATOM | 1869 | NE2 | GLN | 146 | 22.200 | 84.559 | 27.720 | 1.00 | 38.82 | B |
| | ATOM | 1870 | HE21 | GLN | 146 | 21.354 | 84.268 | 28.120 | 1.00 | 0.00 | B |
| | ATOM | 1871 | HE22 | GLN | 146 | 22.239 | 85.092 | 26.900 | 1.00 | 0.00 | B |
| 40 | ATOM | 1872 | C | GLN | 146 | 23.862 | 79.804 | 30.023 | 1.00 | 27.45 | B |
| | ATOM | 1873 | O | GLN | 146 | 24.525 | 79.400 | 29.079 | 1.00 | 22.32 | B |
| | ATOM | 1874 | N | LEU | 147 | 22.965 | 79.050 | 30.622 | 1.00 | 27.23 | B |
| | ATOM | 1875 | H | LEU | 147 | 22.423 | 79.419 | 31.350 | 1.00 | 0.00 | B |
| | ATOM | 1876 | CA | LEU | 147 | 22.776 | 77.675 | 30.211 | 1.00 | 28.64 | B |
| 45 | ATOM | 1877 | CB | LEU | 147 | 23.538 | 76.760 | 31.165 | 1.00 | 27.79 | B |
| | ATOM | 1878 | CG | LEU | 147 | 24.667 | 75.818 | 30.759 | 1.00 | 27.05 | B |
| | ATOM | 1879 | CD1 | LEU | 147 | 25.208 | 76.106 | 29.374 | 1.00 | 24.90 | B |
| | ATOM | 1880 | CD2 | LEU | 147 | 25.742 | 75.956 | 31.812 | 1.00 | 24.14 | B |
| | ATOM | 1881 | C | LEU | 147 | 21.302 | 77.303 | 30.261 | 1.00 | 28.16 | B |
| 50 | ATOM | 1882 | O | LEU | 147 | 20.576 | 77.731 | 31.150 | 1.00 | 25.85 | B |
| | ATOM | 1883 | N | ASP | 148 | 20.872 | 76.502 | 29.297 | 1.00 | 27.82 | B |
| | ATOM | 1884 | H | ASP | 148 | 21.489 | 76.235 | 28.585 | 1.00 | 0.00 | B |
| | ATOM | 1885 | CA | ASP | 148 | 19.506 | 76.019 | 29.279 | 1.00 | 22.46 | B |
| | ATOM | 1886 | CB | ASP | 148 | 18.920 | 76.112 | 27.881 | 1.00 | 20.10 | B |
| 55 | ATOM | 1887 | CG | ASP | 148 | 18.424 | 77.504 | 27.561 | 1.00 | 12.21 | B |
| | ATOM | 1888 | OD1 | ASP | 148 | 18.422 | 77.881 | 26.375 | 1.00 | 14.78 | B |
| | ATOM | 1889 | OD2 | ASP | 148 | 18.040 | 78.216 | 28.494 | 1.00 | 13.58 | B |
| | ATOM | 1890 | C | ASP | 148 | 19.703 | 74.568 | 29.680 | 1.00 | 21.73 | B |
| | ATOM | 1891 | O | ASP | 148 | 20.389 | 73.822 | 28.986 | 1.00 | 23.66 | B |
| 60 | ATOM | 1892 | N | ILE | 149 | 19.138 | 74.190 | 30.822 | 1.00 | 17.82 | B |
| | ATOM | 1893 | H | ILE | 149 | 18.603 | 74.833 | 31.327 | 1.00 | 0.00 | B |
| | ATOM | 1894 | CA | ILE | 149 | 19.296 | 72.838 | 31.332 | 1.00 | 14.75 | B |
| | ATOM | 1895 | CB | ILE | 149 | 19.901 | 72.847 | 32.752 | 1.00 | 15.94 | B |
| | ATOM | 1896 | CG2 | ILE | 149 | 20.143 | 71.431 | 33.218 | 1.00 | 8.68 | B |
| 65 | ATOM | 1897 | CG1 | ILE | 149 | 21.192 | 73.685 | 32.788 | 1.00 | 13.92 | B |
| | ATOM | 1898 | CD1 | ILE | 149 | 21.672 | 73.954 | 34.217 | 1.00 | 7.01 | B |
| | ATOM | 1899 | C | ILE | 149 | 17.977 | 72.076 | 31.427 | 1.00 | 19.66 | B |
| | ATOM | 1900 | O | ILE | 149 | 16.969 | 72.581 | 31.935 | 1.00 | 17.11 | B |
| | ATOM | 1901 | N | VAL | 150 | 18.008 | 70.843 | 30.959 | 1.00 | 15.39 | B |
| 70 | ATOM | 1902 | H | VAL | 150 | 18.833 | 70.497 | 30.565 | 1.00 | 0.00 | B |
| | ATOM | 1903 | CA | VAL | 150 | 16.847 | 69.992 | 31.017 | 1.00 | 14.24 | B |
| | ATOM | 1904 | CB | VAL | 150 | 16.399 | 69.565 | 29.612 | 1.00 | 18.62 | B |
| | ATOM | 1905 | CG1 | VAL | 150 | 15.323 | 68.478 | 29.707 | 1.00 | 11.48 | B |
| | ATOM | 1906 | CG2 | VAL | 150 | 15.861 | 70.773 | 28.869 | 1.00 | 14.10 | B |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| | ATOM | 1907 | C | VAL | 150 | 17.193 | 68.760 | 31.837 | 1.00 | 13.47 | B |
| | ATOM | 1908 | O | VAL | 150 | 18.166 | 68.050 | 31.558 | 1.00 | 16.28 | B |
| | ATOM | 1909 | N | ILE | 151 | 16.390 | 68.534 | 32.864 | 1.00 | 13.89 | B |
| 5 | ATOM | 1910 | H | ILE | 151 | 15.666 | 69.164 | 33.048 | 1.00 | 0.00 | B |
| | ATOM | 1911 | CA | ILE | 151 | 16.554 | 67.384 | 33.725 | 1.00 | 12.32 | B |
| | ATOM | 1912 | CB | ILE | 151 | 16.146 | 67.712 | 35.160 | 1.00 | 8.15 | B |
| | ATOM | 1913 | CG2 | ILE | 151 | 16.359 | 66.524 | 36.033 | 1.00 | 4.81 | B |
| | ATOM | 1914 | CG1 | ILE | 151 | 16.907 | 68.934 | 35.668 | 1.00 | 15.50 | B |
| 10 | ATOM | 1915 | CD1 | ILE | 151 | 16.390 | 69.451 | 37.017 | 1.00 | 16.51 | B |
| | ATOM | 1916 | C | ILE | 151 | 15.625 | 66.309 | 33.174 | 1.00 | 12.57 | B |
| | ATOM | 1917 | O | ILE | 151 | 14.448 | 66.548 | 32.988 | 1.00 | 15.95 | B |
| | ATOM | 1918 | N | VAL | 152 | 16.184 | 65.141 | 32.869 | 1.00 | 16.00 | B |
| | ATOM | 1919 | H | VAL | 152 | 17.150 | 65.032 | 32.993 | 1.00 | 0.00 | B |
| 15 | ATOM | 1920 | CA | VAL | 152 | 15.410 | 64.009 | 32.354 | 1.00 | 14.98 | B |
| | ATOM | 1921 | CB | VAL | 152 | 16.082 | 63.397 | 31.106 | 1.00 | 15.24 | B |
| | ATOM | 1922 | CG1 | VAL | 152 | 15.209 | 62.279 | 30.531 | 1.00 | 10.15 | B |
| | ATOM | 1923 | CG2 | VAL | 152 | 16.313 | 64.500 | 30.056 | 1.00 | 7.29 | B |
| | ATOM | 1924 | C | VAL | 152 | 15.438 | 63.052 | 33.532 | 1.00 | 19.19 | B |
| 20 | ATOM | 1925 | O | VAL | 152 | 16.459 | 62.414 | 33.835 | 1.00 | 16.07 | B |
| | ATOM | 1926 | N | LEU | 153 | 14.297 | 62.976 | 34.200 | 1.00 | 15.97 | B |
| | ATOM | 1927 | H | LEU | 153 | 13.519 | 63.456 | 33.851 | 1.00 | 0.00 | B |
| | ATOM | 1928 | CA | LEU | 153 | 14.150 | 62.211 | 35.414 | 1.00 | 13.99 | B |
| | ATOM | 1929 | CB | LEU | 153 | 13.530 | 63.131 | 36.474 | 1.00 | 15.97 | B |
| 25 | ATOM | 1930 | CG | LEU | 153 | 12.764 | 62.553 | 37.658 | 1.00 | 17.17 | B |
| | ATOM | 1931 | CD1 | LEU | 153 | 13.616 | 61.536 | 38.376 | 1.00 | 23.41 | B |
| | ATOM | 1932 | CD2 | LEU | 153 | 12.367 | 63.672 | 38.599 | 1.00 | 15.08 | B |
| | ATOM | 1933 | C | LEU | 153 | 13.362 | 60.924 | 35.309 | 1.00 | 17.91 | B |
| | ATOM | 1934 | O | LEU | 153 | 12.214 | 60.923 | 34.870 | 1.00 | 23.80 | B |
| 30 | ATOM | 1935 | N | ASP | 154 | 14.002 | 59.832 | 35.723 | 1.00 | 19.62 | B |
| | ATOM | 1936 | H | ASP | 154 | 14.918 | 59.927 | 36.051 | 1.00 | 0.00 | B |
| | ATOM | 1937 | CA | ASP | 154 | 13.397 | 58.504 | 35.709 | 1.00 | 19.43 | B |
| | ATOM | 1938 | CB | ASP | 154 | 14.461 | 57.432 | 35.966 | 1.00 | 17.84 | B |
| | ATOM | 1939 | CG | ASP | 154 | 13.912 | 56.021 | 35.831 | 1.00 | 27.80 | B |
| 35 | ATOM | 1940 | OD1 | ASP | 154 | 12.725 | 55.871 | 35.461 | 1.00 | 28.40 | B |
| | ATOM | 1941 | OD2 | ASP | 154 | 14.667 | 55.059 | 36.094 | 1.00 | 28.69 | B |
| | ATOM | 1942 | C | ASP | 154 | 12.351 | 58.419 | 36.804 | 1.00 | 18.93 | B |
| | ATOM | 1943 | O | ASP | 154 | 12.698 | 58.429 | 37.993 | 1.00 | 15.86 | B |
| 40 | ATOM | 1944 | N | GLY | 155 | 11.080 | 58.328 | 36.407 | 1.00 | 18.75 | B |
| | ATOM | 1945 | H | GLY | 155 | 10.873 | 58.317 | 35.453 | 1.00 | 0.00 | B |
| | ATOM | 1946 | CA | GLY | 155 | 10.012 | 58.247 | 37.382 | 1.00 | 15.14 | B |
| | ATOM | 1947 | C | GLY | 155 | 9.479 | 56.842 | 37.537 | 1.00 | 19.82 | B |
| | ATOM | 1948 | O | GLY | 155 | 8.308 | 56.668 | 37.882 | 1.00 | 14.58 | B |
| | ATOM | 1949 | N | SER | 156 | 10.342 | 55.854 | 37.280 | 1.00 | 18.73 | B |
| 45 | ATOM | 1950 | H | SER | 156 | 11.250 | 56.096 | 37.000 | 1.00 | 0.00 | B |
| | ATOM | 1951 | CA | SER | 156 | 10.008 | 54.434 | 37.396 | 1.00 | 17.78 | B |
| | ATOM | 1952 | CB | SER | 156 | 11.217 | 53.559 | 36.993 | 1.00 | 23.82 | B |
| | ATOM | 1953 | OG | SER | 156 | 12.195 | 53.479 | 38.040 | 1.00 | 34.45 | B |
| | ATOM | 1954 | HG | SER | 156 | 12.517 | 54.359 | 38.245 | 1.00 | 0.00 | B |
| 50 | ATOM | 1955 | C | SER | 156 | 9.581 | 54.127 | 38.826 | 1.00 | 14.28 | B |
| | ATOM | 1956 | O | SER | 156 | 9.531 | 55.014 | 39.675 | 1.00 | 16.84 | B |
| | ATOM | 1957 | N | ASN | 157 | 9.298 | 52.866 | 39.113 | 1.00 | 15.15 | B |
| | ATOM | 1958 | H | ASN | 157 | 9.411 | 52.173 | 38.428 | 1.00 | 0.00 | B |
| | ATOM | 1959 | CA | ASN | 157 | 8.820 | 52.507 | 40.443 | 1.00 | 13.34 | B |
| 55 | ATOM | 1960 | CB | ASN | 157 | 7.869 | 51.305 | 40.353 | 1.00 | 16.24 | B |
| | ATOM | 1961 | CG | ASN | 157 | 6.634 | 51.580 | 39.529 | 1.00 | 20.72 | B |
| | ATOM | 1962 | OD1 | ASN | 157 | 5.997 | 50.643 | 39.036 | 1.00 | 27.20 | B |
| | ATOM | 1963 | ND2 | ASN | 157 | 6.273 | 52.859 | 39.374 | 1.00 | 18.41 | B |
| | ATOM | 1964 | HD21 | ASN | 157 | 6.805 | 53.570 | 39.787 | 1.00 | 0.00 | B |
| 60 | ATOM | 1965 | HD22 | ASN | 157 | 5.473 | 53.041 | 38.841 | 1.00 | 0.00 | B |
| | ATOM | 1966 | C | ASN | 157 | 9.865 | 52.190 | 41.511 | 1.00 | 16.46 | B |
| | ATOM | 1967 | O | ASN | 157 | 9.517 | 52.117 | 42.693 | 1.00 | 20.71 | B |
| | ATOM | 1968 | N | SER | 158 | 11.127 | 52.030 | 41.132 | 1.00 | 15.18 | B |
| | ATOM | 1969 | H | SER | 158 | 11.384 | 52.156 | 40.196 | 1.00 | 0.00 | B |
| 65 | ATOM | 1970 | CA | SER | 158 | 12.151 | 51.654 | 42.127 | 1.00 | 16.23 | B |
| | ATOM | 1971 | CB | SER | 158 | 13.161 | 50.690 | 41.487 | 1.00 | 13.88 | B |
| | ATOM | 1972 | OG | SER | 158 | 13.678 | 51.221 | 40.296 | 1.00 | 15.34 | B |
| | ATOM | 1973 | HG | SER | 158 | 14.121 | 52.052 | 40.478 | 1.00 | 0.00 | B |
| | ATOM | 1974 | C | SER | 158 | 12.911 | 52.713 | 42.948 | 1.00 | 17.21 | B |
| 70 | ATOM | 1975 | O | SER | 158 | 13.395 | 52.397 | 44.046 | 1.00 | 16.37 | B |
| | ATOM | 1976 | N | ILE | 159 | 13.061 | 53.938 | 42.446 | 1.00 | 22.58 | B |
| | ATOM | 1977 | H | ILE | 159 | 12.726 | 54.145 | 41.550 | 1.00 | 0.00 | B |
| | ATOM | 1978 | CA | ILE | 159 | 13.733 | 54.975 | 43.241 | 1.00 | 22.49 | B |
| | ATOM | 1979 | CB | ILE | 159 | 13.674 | 56.360 | 42.566 | 1.00 | 24.48 | B |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 1980 | CG2 | ILE | 159 | 14.718 | 57.288 | 43.176 | 1.00 | 24.15 | B |
| | ATOM | 1981 | CG1 | ILE | 159 | 13.812 | 56.209 | 41.057 | 1.00 | 32.59 | B |
| | ATOM | 1982 | CD1 | ILE | 159 | 12.470 | 56.393 | 40.303 | 1.00 | 20.06 | B |
| | ATOM | 1983 | C | ILE | 159 | 12.778 | 55.028 | 44.407 | 1.00 | 24.33 | B |
| | ATOM | 1984 | O | ILE | 159 | 11.724 | 55.618 | 44.285 | 1.00 | 17.55 | B |
| 10 | ATOM | 1985 | N | TYR | 160 | 13.099 | 54.420 | 45.541 | 1.00 | 32.15 | B |
| | ATOM | 1986 | H | TYR | 160 | 13.965 | 53.980 | 45.664 | 1.00 | 0.00 | B |
| | ATOM | 1987 | CA | TYR | 160 | 12.097 | 54.447 | 46.585 | 1.00 | 31.82 | B |
| | ATOM | 1988 | CB | TYR | 160 | 12.267 | 53.324 | 47.597 | 1.00 | 26.96 | B |
| | ATOM | 1989 | CG | TYR | 160 | 11.253 | 53.490 | 48.725 | 1.00 | 25.65 | B |
| 15 | ATOM | 1990 | CD1 | TYR | 160 | 9.926 | 53.897 | 48.457 | 1.00 | 24.26 | B |
| | ATOM | 1991 | CE1 | TYR | 160 | 9.022 | 54.114 | 49.484 | 1.00 | 18.27 | B |
| | ATOM | 1992 | CD2 | TYR | 160 | 11.623 | 53.306 | 50.041 | 1.00 | 20.35 | B |
| | ATOM | 1993 | CE2 | TYR | 160 | 10.729 | 53.519 | 51.072 | 1.00 | 22.84 | B |
| | ATOM | 1994 | CZ | TYR | 160 | 9.441 | 53.917 | 50.791 | 1.00 | 14.51 | B |
| 20 | ATOM | 1995 | OH | TYR | 160 | 8.598 | 54.099 | 51.840 | 1.00 | 23.91 | B |
| | ATOM | 1996 | HH | TYR | 160 | 9.063 | 53.916 | 52.661 | 1.00 | 0.00 | B |
| | ATOM | 1997 | C | TYR | 160 | 11.880 | 55.733 | 47.356 | 1.00 | 37.48 | B |
| | ATOM | 1998 | O | TYR | 160 | 10.799 | 56.335 | 47.262 | 1.00 | 44.11 | B |
| | ATOM | 1999 | N | PRO | 161 | 12.855 | 56.167 | 48.158 | 1.00 | 31.96 | B |
| 25 | ATOM | 2000 | CD | PRO | 161 | 14.215 | 55.743 | 48.529 | 1.00 | 22.44 | B |
| | ATOM | 2001 | CA | PRO | 161 | 12.466 | 57.408 | 48.822 | 1.00 | 28.82 | B |
| | ATOM | 2002 | CB | PRO | 161 | 13.575 | 57.639 | 49.856 | 1.00 | 31.11 | B |
| | ATOM | 2003 | CG | PRO | 161 | 14.337 | 56.332 | 49.902 | 1.00 | 29.58 | B |
| | ATOM | 2004 | C | PRO | 161 | 12.414 | 58.464 | 47.729 | 1.00 | 23.46 | B |
| 30 | ATOM | 2005 | O | PRO | 161 | 13.452 | 58.977 | 47.298 | 1.00 | 18.53 | B |
| | ATOM | 2006 | N | TRP | 162 | 11.204 | 58.741 | 47.246 | 1.00 | 23.04 | B |
| | ATOM | 2007 | H | TRP | 162 | 10.424 | 58.275 | 47.612 | 1.00 | 0.00 | B |
| | ATOM | 2008 | CA | TRP | 162 | 11.019 | 59.719 | 46.184 | 1.00 | 20.85 | B |
| | ATOM | 2009 | CB | TRP | 162 | 9.565 | 59.743 | 45.720 | 1.00 | 24.84 | B |
| 35 | ATOM | 2010 | CG | TRP | 162 | 9.344 | 60.700 | 44.583 | 1.00 | 15.34 | B |
| | ATOM | 2011 | CD2 | TRP | 162 | 9.779 | 60.531 | 43.229 | 1.00 | 17.68 | B |
| | ATOM | 2012 | CE2 | TRP | 162 | 9.364 | 61.679 | 42.516 | 1.00 | 13.50 | B |
| | ATOM | 2013 | CE3 | TRP | 162 | 10.474 | 59.531 | 42.545 | 1.00 | 12.30 | B |
| | ATOM | 2014 | CD1 | TRP | 162 | 8.704 | 61.897 | 44.640 | 1.00 | 12.84 | B |
| 40 | ATOM | 2015 | NE1 | TRP | 162 | 8.712 | 62.491 | 43.399 | 1.00 | 14.37 | B |
| | ATOM | 2016 | HE1 | TRP | 162 | 8.323 | 63.357 | 43.175 | 1.00 | 0.00 | B |
| | ATOM | 2017 | CZ2 | TRP | 162 | 9.625 | 61.847 | 41.158 | 1.00 | 14.57 | B |
| | ATOM | 2018 | CZ3 | TRP | 162 | 10.732 | 59.699 | 41.198 | 1.00 | 13.59 | B |
| | ATOM | 2019 | CH2 | TRP | 162 | 10.307 | 60.853 | 40.517 | 1.00 | 10.94 | B |
| 45 | ATOM | 2020 | C | TRP | 162 | 11.431 | 61.091 | 46.692 | 1.00 | 21.81 | B |
| | ATOM | 2021 | O | TRP | 162 | 12.010 | 61.884 | 45.969 | 1.00 | 16.84 | B |
| | ATOM | 2022 | N | GLU | 163 | 11.135 | 61.363 | 47.952 | 1.00 | 25.91 | B |
| | ATOM | 2023 | H | GLU | 163 | 10.665 | 60.699 | 48.497 | 1.00 | 0.00 | B |
| | ATOM | 2024 | CA | GLU | 163 | 11.506 | 62.644 | 48.524 | 1.00 | 33.12 | B |
| 50 | ATOM | 2025 | CB | GLU | 163 | 11.066 | 62.721 | 49.993 | 1.00 | 36.71 | B |
| | ATOM | 2026 | CG | GLU | 163 | 11.646 | 61.637 | 50.888 | 1.00 | 47.66 | B |
| | ATOM | 2027 | CD | GLU | 163 | 10.848 | 61.447 | 52.173 | 1.00 | 55.21 | B |
| | ATOM | 2028 | OE1 | GLU | 163 | 11.446 | 61.522 | 53.270 | 1.00 | 57.76 | B |
| | ATOM | 2029 | OE2 | GLU | 163 | 9.620 | 61.221 | 52.088 | 1.00 | 59.92 | B |
| 55 | ATOM | 2030 | C | GLU | 163 | 13.013 | 62.848 | 48.418 | 1.00 | 31.56 | B |
| | ATOM | 2031 | O | GLU | 163 | 13.496 | 63.980 | 48.447 | 1.00 | 28.76 | B |
| | ATOM | 2032 | N | SER | 164 | 13.748 | 61.747 | 48.270 | 1.00 | 31.75 | B |
| | ATOM | 2033 | H | SER | 164 | 13.295 | 60.879 | 48.215 | 1.00 | 0.00 | B |
| | ATOM | 2034 | CA | SER | 164 | 15.213 | 61.788 | 48.181 | 1.00 | 31.88 | B |
| 60 | ATOM | 2035 | CB | SER | 164 | 15.795 | 60.399 | 48.470 | 1.00 | 31.21 | B |
| | ATOM | 2036 | OG | SER | 164 | 15.996 | 60.221 | 49.864 | 1.00 | 32.68 | B |
| | ATOM | 2037 | HG | SER | 164 | 16.606 | 60.887 | 50.185 | 1.00 | 0.00 | B |
| | ATOM | 2038 | C | SER | 164 | 15.751 | 62.289 | 46.845 | 1.00 | 29.05 | B |
| | ATOM | 2039 | O | SER | 164 | 16.820 | 62.890 | 46.782 | 1.00 | 29.91 | B |
| 65 | ATOM | 2040 | N | VAL | 165 | 15.030 | 61.998 | 45.772 | 1.00 | 22.58 | B |
| | ATOM | 2041 | H | VAL | 165 | 14.209 | 61.472 | 45.867 | 1.00 | 0.00 | B |
| | ATOM | 2042 | CA | VAL | 165 | 15.443 | 62.454 | 44.462 | 1.00 | 26.86 | B |
| | ATOM | 2043 | CB | VAL | 165 | 14.761 | 61.610 | 43.333 | 1.00 | 30.69 | B |
| | ATOM | 2044 | CG1 | VAL | 165 | 13.791 | 62.460 | 42.533 | 1.00 | 27.74 | B |
| 70 | ATOM | 2045 | CG2 | VAL | 165 | 15.825 | 61.022 | 42.411 | 1.00 | 33.05 | B |
| | ATOM | 2046 | C | VAL | 165 | 15.029 | 63.926 | 44.386 | 1.00 | 27.11 | B |
| | ATOM | 2047 | O | VAL | 165 | 15.746 | 64.762 | 43.843 | 1.00 | 23.73 | B |
| | ATOM | 2048 | N | ILE | 166 | 13.860 | 64.238 | 44.936 | 1.00 | 26.45 | B |
| | ATOM | 2049 | H | ILE | 166 | 13.308 | 63.536 | 45.338 | 1.00 | 0.00 | B |
| | ATOM | 2050 | CA | ILE | 166 | 13.388 | 65.618 | 44.943 | 1.00 | 21.89 | B |
| | ATOM | 2051 | CB | ILE | 166 | 11.931 | 65.706 | 45.407 | 1.00 | 24.39 | B |
| | ATOM | 2052 | CG2 | ILE | 166 | 11.469 | 67.157 | 45.379 | 1.00 | 22.62 | B |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 2053 | CG1 | ILE | 166 | 11.047 | 64.822 | 44.505 | 1.00 | 28.66 | B |
| | ATOM | 2054 | CD1 | ILE | 166 | 11.350 | 64.929 | 42.999 | 1.00 | 20.77 | B |
| | ATOM | 2055 | C | ILE | 166 | 14.283 | 66.471 | 45.842 | 1.00 | 18.82 | B |
| | ATOM | 2056 | O | ILE | 166 | 14.476 | 67.651 | 45.577 | 1.00 | 18.46 | B |
| | ATOM | 2057 | N | ALA | 167 | 14.828 | 65.882 | 46.904 | 1.00 | 12.61 | B |
| 10 | ATOM | 2058 | H | ALA | 167 | 14.615 | 64.949 | 47.105 | 1.00 | 0.00 | B |
| | ATOM | 2059 | CA | ALA | 167 | 15.750 | 66.625 | 47.768 | 1.00 | 14.63 | B |
| | ATOM | 2060 | CB | ALA | 167 | 16.054 | 65.836 | 49.048 | 1.00 | 15.91 | B |
| | ATOM | 2061 | C | ALA | 167 | 17.045 | 66.847 | 46.961 | 1.00 | 15.69 | B |
| | ATOM | 2062 | O | ALA | 167 | 17.647 | 67.906 | 47.036 | 1.00 | 17.79 | B |
| 15 | ATOM | 2063 | N | PHE | 168 | 17.450 | 65.842 | 46.181 | 1.00 | 14.44 | B |
| | ATOM | 2064 | H | PHE | 168 | 16.926 | 65.014 | 46.166 | 1.00 | 0.00 | B |
| | ATOM | 2065 | CA | PHE | 168 | 18.656 | 65.936 | 45.346 | 1.00 | 14.68 | B |
| | ATOM | 2066 | CB | PHE | 168 | 18.878 | 64.608 | 44.615 | 1.00 | 12.59 | B |
| | ATOM | 2067 | CG | PHE | 168 | 19.832 | 64.680 | 43.444 | 1.00 | 20.18 | B |
| 20 | ATOM | 2068 | CD1 | PHE | 168 | 19.355 | 64.609 | 42.134 | 1.00 | 17.37 | B |
| | ATOM | 2069 | CD2 | PHE | 168 | 21.211 | 64.759 | 43.645 | 1.00 | 16.50 | B |
| | ATOM | 2070 | CE1 | PHE | 168 | 20.226 | 64.606 | 41.047 | 1.00 | 18.84 | B |
| | ATOM | 2071 | CE2 | PHE | 168 | 22.092 | 64.760 | 42.564 | 1.00 | 14.29 | B |
| | ATOM | 2072 | CZ | PHE | 168 | 21.599 | 64.680 | 41.263 | 1.00 | 15.75 | B |
| 25 | ATOM | 2073 | C | PHE | 168 | 18.501 | 67.066 | 44.336 | 1.00 | 17.90 | B |
| | ATOM | 2074 | O | PHE | 168 | 19.420 | 67.847 | 44.114 | 1.00 | 19.14 | B |
| | ATOM | 2075 | N | LEU | 169 | 17.328 | 67.148 | 43.719 | 1.00 | 18.88 | B |
| | ATOM | 2076 | H | LEU | 169 | 16.627 | 66.494 | 43.929 | 1.00 | 0.00 | B |
| | ATOM | 2077 | CA | LEU | 169 | 17.068 | 68.187 | 42.745 | 1.00 | 16.96 | B |
| 30 | ATOM | 2078 | CB | LEU | 169 | 15.779 | 67.885 | 41.984 | 1.00 | 19.20 | B |
| | ATOM | 2079 | CG | LEU | 169 | 15.843 | 66.692 | 41.022 | 1.00 | 14.34 | B |
| | ATOM | 2080 | CD1 | LEU | 169 | 14.476 | 66.482 | 40.428 | 1.00 | 16.09 | B |
| | ATOM | 2081 | CD2 | LEU | 169 | 16.864 | 66.920 | 39.926 | 1.00 | 14.01 | B |
| | ATOM | 2082 | C | LEU | 169 | 16.977 | 69.558 | 43.407 | 1.00 | 19.79 | B |
| 35 | ATOM | 2083 | O | LEU | 169 | 17.443 | 70.547 | 42.844 | 1.00 | 26.07 | B |
| | ATOM | 2084 | N | ASN | 170 | 16.377 | 69.617 | 44.593 | 1.00 | 21.05 | B |
| | ATOM | 2085 | H | ASN | 170 | 16.011 | 68.795 | 44.984 | 1.00 | 0.00 | B |
| | ATOM | 2086 | CA | ASN | 170 | 16.249 | 70.875 | 45.332 | 1.00 | 22.16 | B |
| | ATOM | 2087 | CB | ASN | 170 | 15.473 | 70.655 | 46.630 | 1.00 | 27.93 | B |
| 40 | ATOM | 2088 | CG | ASN | 170 | 15.617 | 71.834 | 47.611 | 1.00 | 32.39 | B |
| | ATOM | 2089 | OD1 | ASN | 170 | 16.661 | 72.003 | 48.257 | 1.00 | 29.22 | B |
| | ATOM | 2090 | ND2 | ASN | 170 | 14.572 | 72.643 | 47.718 | 1.00 | 25.77 | B |
| | ATOM | 2091 | HD21 | ASN | 170 | 13.765 | 72.473 | 47.191 | 1.00 | 0.00 | B |
| | ATOM | 2092 | HD22 | ASN | 170 | 14.648 | 73.396 | 48.340 | 1.00 | 0.00 | B |
| 45 | ATOM | 2093 | C | ASN | 170 | 17.609 | 71.498 | 45.668 | 1.00 | 24.44 | B |
| | ATOM | 2094 | O | ASN | 170 | 17.832 | 72.689 | 45.426 | 1.00 | 24.64 | B |
| | ATOM | 2095 | N | ASP | 171 | 18.509 | 70.684 | 46.223 | 1.00 | 22.99 | B |
| | ATOM | 2096 | H | ASP | 171 | 18.262 | 69.748 | 46.378 | 1.00 | 0.00 | B |
| | ATOM | 2097 | CA | ASP | 171 | 19.855 | 71.128 | 46.610 | 1.00 | 20.63 | B |
| 50 | ATOM | 2098 | CB | ASP | 171 | 20.593 | 70.014 | 47.360 | 1.00 | 20.85 | B |
| | ATOM | 2099 | CG | ASP | 171 | 19.869 | 69.585 | 48.619 | 1.00 | 29.81 | B |
| | ATOM | 2100 | OD1 | ASP | 171 | 19.031 | 70.371 | 49.124 | 1.00 | 25.40 | B |
| | ATOM | 2101 | OD2 | ASP | 171 | 20.131 | 68.465 | 49.104 | 1.00 | 29.96 | B |
| | ATOM | 2102 | C | ASP | 171 | 20.685 | 71.544 | 45.416 | 1.00 | 22.06 | B |
| 55 | ATOM | 2103 | O | ASP | 171 | 21.537 | 72.431 | 45.519 | 1.00 | 26.11 | B |
| | ATOM | 2104 | N | LEU | 172 | 20.447 | 70.876 | 44.292 | 1.00 | 19.55 | B |
| | ATOM | 2105 | H | LEU | 172 | 19.776 | 70.165 | 44.301 | 1.00 | 0.00 | B |
| | ATOM | 2106 | CA | LEU | 172 | 21.146 | 71.162 | 43.050 | 1.00 | 20.55 | B |
| | ATOM | 2107 | CB | LEU | 172 | 20.866 | 70.044 | 42.056 | 1.00 | 25.39 | B |
| 60 | ATOM | 2108 | CG | LEU | 172 | 21.889 | 69.703 | 40.978 | 1.00 | 23.87 | B |
| | ATOM | 2109 | CD1 | LEU | 172 | 21.174 | 68.935 | 39.874 | 1.00 | 26.42 | B |
| | ATOM | 2110 | CD2 | LEU | 172 | 22.543 | 70.947 | 40.435 | 1.00 | 32.73 | B |
| | ATOM | 2111 | C | LEU | 172 | 20.697 | 72.484 | 42.428 | 1.00 | 20.44 | B |
| | ATOM | 2112 | O | LEU | 172 | 21.518 | 73.313 | 42.014 | 1.00 | 21.12 | B |
| 65 | ATOM | 2113 | N | LEU | 173 | 19.383 | 72.646 | 42.343 | 1.00 | 18.93 | B |
| | ATOM | 2114 | H | LEU | 173 | 18.803 | 71.938 | 42.694 | 1.00 | 0.00 | B |
| | ATOM | 2115 | CA | LEU | 173 | 18.761 | 73.826 | 41.755 | 1.00 | 21.30 | B |
| | ATOM | 2116 | CB | LEU | 173 | 17.248 | 73.588 | 41.573 | 1.00 | 20.45 | B |
| | ATOM | 2117 | CG | LEU | 173 | 16.850 | 72.431 | 40.649 | 1.00 | 20.49 | B |
| 70 | ATOM | 2118 | CD1 | LEU | 173 | 15.418 | 72.019 | 40.926 | 1.00 | 22.02 | B |
| | ATOM | 2119 | CD2 | LEU | 173 | 16.999 | 72.855 | 39.197 | 1.00 | 25.70 | B |
| | ATOM | 2120 | C | LEU | 173 | 18.966 | 75.081 | 42.583 | 1.00 | 18.86 | B |
| | ATOM | 2121 | O | LEU | 173 | 19.266 | 76.146 | 42.046 | 1.00 | 16.41 | B |
| | ATOM | 2122 | N | LYS | 174 | 18.799 | 74.953 | 43.894 | 1.00 | 21.55 | B |
| | ATOM | 2123 | H | LYS | 174 | 18.581 | 74.076 | 44.275 | 1.00 | 0.00 | B |
| | ATOM | 2124 | CA | LYS | 174 | 18.943 | 76.107 | 44.765 | 1.00 | 23.18 | B |
| | ATOM | 2125 | CB | LYS | 174 | 18.648 | 75.717 | 46.216 | 1.00 | 26.28 | B |

| | | | | | | | | | | | |
|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|---|
| | ATOM | 2126 | CG | LYS | 174 | 19.830 | 75.202 | 47.026 | 1.00 | 29.25 | B |
| | ATOM | 2127 | CD | LYS | 174 | 19.306 | 74.550 | 48.304 | 1.00 | 28.29 | B |
| | ATOM | 2128 | CE | LYS | 174 | 20.399 | 73.886 | 49.111 | 1.00 | 19.54 | B |
| | ATOM | 2129 | NZ | LYS | 174 | 19.815 | 73.374 | 50.359 | 1.00 | 21.14 | B |
| 5 | ATOM | 2130 | HZ1 | LYS | 174 | 19.069 | 72.682 | 50.131 | 1.00 | 0.00 | B |
| | ATOM | 2131 | HZ2 | LYS | 174 | 19.398 | 74.161 | 50.895 | 1.00 | 0.00 | B |
| | ATOM | 2132 | HZ3 | LYS | 174 | 20.551 | 72.915 | 50.926 | 1.00 | 0.00 | B |
| | ATOM | 2133 | C | LYS | 174 | 20.288 | 76.818 | 44.661 | 1.00 | 22.91 | B |
| | ATOM | 2134 | O | LYS | 174 | 20.420 | 77.948 | 45.110 | 1.00 | 22.73 | B |
| 10 | ATOM | 2135 | N | ALA | 175 | 21.279 | 76.173 | 44.059 | 1.00 | 23.45 | B |
| | ATOM | 2136 | H | ALA | 175 | 21.134 | 75.270 | 43.705 | 1.00 | 0.00 | B |
| | ATOM | 2137 | CA | ALA | 175 | 22.589 | 76.807 | 43.929 | 1.00 | 26.35 | B |
| | ATOM | 2138 | CB | ALA | 175 | 23.694 | 75.755 | 43.981 | 1.00 | 22.79 | B |
| | ATOM | 2139 | C | ALA | 175 | 22.730 | 77.649 | 42.658 | 1.00 | 26.76 | B |
| 15 | ATOM | 2140 | O | ALA | 175 | 23.651 | 78.460 | 42.539 | 1.00 | 29.91 | B |
| | ATOM | 2141 | N | MET | 176 | 21.821 | 77.470 | 41.710 | 1.00 | 25.18 | B |
| | ATOM | 2142 | H | MET | 176 | 21.098 | 76.822 | 41.845 | 1.00 | 0.00 | B |
| | ATOM | 2143 | CA | MET | 176 | 21.888 | 78.226 | 40.467 | 1.00 | 24.53 | B |
| | ATOM | 2144 | CB | MET | 176 | 21.253 | 77.418 | 39.336 | 1.00 | 22.97 | B |
| 20 | ATOM | 2145 | CG | MET | 176 | 21.779 | 76.003 | 39.265 | 1.00 | 22.20 | B |
| | ATOM | 2146 | SD | MET | 176 | 20.923 | 74.945 | 38.090 | 1.00 | 24.68 | B |
| | ATOM | 2147 | CE | MET | 176 | 22.045 | 73.494 | 38.136 | 1.00 | 19.10 | B |
| | ATOM | 2148 | C | MET | 176 | 21.227 | 79.595 | 40.548 | 1.00 | 24.31 | B |
| | ATOM | 2149 | O | MET | 176 | 20.618 | 79.958 | 41.554 | 1.00 | 31.33 | B |
| 25 | ATOM | 2150 | N | ASP | 177 | 21.365 | 80.354 | 39.469 | 1.00 | 24.61 | B |
| | ATOM | 2151 | H | ASP | 177 | 21.887 | 80.004 | 38.717 | 1.00 | 0.00 | B |
| | ATOM | 2152 | CA | ASP | 177 | 20.777 | 81.678 | 39.355 | 1.00 | 24.49 | B |
| | ATOM | 2153 | CB | ASP | 177 | 21.848 | 82.729 | 39.075 | 1.00 | 30.14 | B |
| | ATOM | 2154 | CG | ASP | 177 | 21.348 | 84.131 | 39.296 | 1.00 | 33.29 | B |
| 30 | ATOM | 2155 | OD1 | ASP | 177 | 22.134 | 84.977 | 39.767 | 1.00 | 37.03 | B |
| | ATOM | 2156 | OD2 | ASP | 177 | 20.160 | 84.388 | 39.000 | 1.00 | 42.39 | B |
| | ATOM | 2157 | C | ASP | 177 | 19.881 | 81.525 | 38.153 | 1.00 | 21.41 | B |
| | ATOM | 2158 | O | ASP | 177 | 20.365 | 81.519 | 37.017 | 1.00 | 20.00 | B |
| | ATOM | 2159 | N | ILE | 178 | 18.581 | 81.390 | 38.407 | 1.00 | 18.68 | B |
| 35 | ATOM | 2160 | H | ILE | 178 | 18.270 | 81.436 | 39.336 | 1.00 | 0.00 | B |
| | ATOM | 2161 | CA | ILE | 178 | 17.610 | 81.169 | 37.350 | 1.00 | 20.35 | B |
| | ATOM | 2162 | CB | ILE | 178 | 16.525 | 80.193 | 37.788 | 1.00 | 24.17 | B |
| | ATOM | 2163 | CG2 | ILE | 178 | 15.745 | 79.714 | 36.559 | 1.00 | 26.64 | B |
| | ATOM | 2164 | CG1 | ILE | 178 | 17.154 | 79.024 | 38.560 | 1.00 | 26.03 | B |
| 40 | ATOM | 2165 | CD1 | ILE | 178 | 17.407 | 77.790 | 37.734 | 1.00 | 21.54 | B |
| | ATOM | 2166 | C | ILE | 178 | 16.916 | 82.410 | 36.840 | 1.00 | 21.48 | B |
| | ATOM | 2167 | O | ILE | 178 | 16.327 | 83.164 | 37.598 | 1.00 | 13.16 | B |
| | ATOM | 2168 | N | GLY | 179 | 16.977 | 82.586 | 35.527 | 1.00 | 23.27 | B |
| | ATOM | 2169 | H | GLY | 179 | 17.457 | 81.937 | 34.974 | 1.00 | 0.00 | B |
| 45 | ATOM | 2170 | CA | GLY | 179 | 16.346 | 83.727 | 34.904 | 1.00 | 24.96 | B |
| | ATOM | 2171 | C | GLY | 179 | 16.621 | 83.775 | 33.414 | 1.00 | 25.44 | B |
| | ATOM | 2172 | O | GLY | 179 | 17.505 | 83.087 | 32.906 | 1.00 | 18.86 | B |
| | ATOM | 2173 | N | PRO | 180 | 15.844 | 84.583 | 32.685 | 1.00 | 27.50 | B |
| | ATOM | 2174 | CD | PRO | 180 | 14.721 | 85.395 | 33.194 | 1.00 | 23.45 | B |
| 50 | ATOM | 2175 | CA | PRO | 180 | 16.006 | 84.725 | 31.240 | 1.00 | 25.34 | B |
| | ATOM | 2176 | CB | PRO | 180 | 14.991 | 85.817 | 30.881 | 1.00 | 28.96 | B |
| | ATOM | 2177 | CG | PRO | 180 | 13.934 | 85.689 | 31.956 | 1.00 | 21.85 | B |
| | ATOM | 2178 | C | PRO | 180 | 17.434 | 85.104 | 30.859 | 1.00 | 21.40 | B |
| | ATOM | 2179 | O | PRO | 180 | 17.889 | 84.771 | 29.780 | 1.00 | 17.19 | B |
| 55 | ATOM | 2180 | N | LYS | 181 | 18.126 | 85.779 | 31.773 | 1.00 | 22.62 | B |
| | ATOM | 2181 | H | LYS | 181 | 17.698 | 85.977 | 32.631 | 1.00 | 0.00 | B |
| | ATOM | 2182 | CA | LYS | 181 | 19.493 | 86.244 | 31.555 | 1.00 | 22.16 | B |
| | ATOM | 2183 | CB | LYS | 181 | 19.628 | 87.682 | 32.050 | 1.00 | 27.02 | B |
| 60 | ATOM | 2184 | CG | LYS | 181 | 18.711 | 88.652 | 31.352 | 1.00 | 32.06 | B |
| | ATOM | 2185 | CD | LYS | 181 | 19.157 | 88.876 | 29.925 | 1.00 | 29.94 | B |
| | ATOM | 2186 | CE | LYS | 181 | 19.909 | 90.182 | 29.788 | 1.00 | 34.20 | B |
| | ATOM | 2187 | NZ | LYS | 181 | 20.167 | 90.503 | 28.357 | 1.00 | 34.68 | B |
| | ATOM | 2188 | HZ1 | LYS | 181 | 19.264 | 90.584 | 27.850 | 1.00 | 0.00 | B |
| | ATOM | 2189 | HZ2 | LYS | 181 | 20.738 | 89.744 | 27.930 | 1.00 | 0.00 | B |
| 65 | ATOM | 2190 | HZ3 | LYS | 181 | 20.685 | 91.402 | 28.291 | 1.00 | 0.00 | B |
| | ATOM | 2191 | C | LYS | 181 | 20.585 | 85.395 | 32.206 | 1.00 | 22.21 | B |
| | ATOM | 2192 | O | LYS | 181 | 21.764 | 85.684 | 32.044 | 1.00 | 20.87 | B |
| | ATOM | 2193 | N | GLN | 182 | 20.194 | 84.379 | 32.958 | 1.00 | 23.88 | B |
| | ATOM | 2194 | H | GLN | 182 | 19.235 | 84.212 | 33.077 | 1.00 | 0.00 | B |
| 70 | ATOM | 2195 | CA | GLN | 182 | 21.156 | 83.498 | 33.616 | 1.00 | 27.46 | B |
| | ATOM | 2196 | CB | GLN | 182 | 21.004 | 83.585 | 35.136 | 1.00 | 31.07 | B |
| | ATOM | 2197 | CG | GLN | 182 | 20.735 | 84.991 | 35.668 | 1.00 | 38.02 | B |
| | ATOM | 2198 | CD | GLN | 182 | 21.886 | 85.950 | 35.421 | 1.00 | 42.63 | B |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| | ATOM | 2199 | OE1 | GLN | 182 | 21.708 | 87.167 | 35.435 | 1.00 | 44.04 | B |
| | ATOM | 2200 | NE2 | GLN | 182 | 23.072 | 85.406 | 35.190 | 1.00 | 43.73 | B |
| | ATOM | 2201 | HE21 | GLN | 182 | 23.171 | 84.431 | 35.184 | 1.00 | 0.00 | B |
| | ATOM | 2202 | HE22 | GLN | 182 | 23.824 | 86.012 | 35.029 | 1.00 | 0.00 | B |
| 5 | ATOM | 2203 | C | GLN | 182 | 20.880 | 82.076 | 33.135 | 1.00 | 26.08 | B |
| | ATOM | 2204 | O | GLN | 182 | 20.806 | 81.835 | 31.926 | 1.00 | 22.28 | B |
| | ATOM | 2205 | N | THR | 183 | 20.732 | 81.132 | 34.058 | 1.00 | 18.41 | B |
| | ATOM | 2206 | H | THR | 183 | 20.823 | 81.350 | 35.010 | 1.00 | 0.00 | B |
| 10 | ATOM | 2207 | CA | THR | 183 | 20.439 | 79.778 | 33.640 | 1.00 | 21.94 | B |
| | ATOM | 2208 | CB | THR | 183 | 21.165 | 78.705 | 34.513 | 1.00 | 27.45 | B |
| | ATOM | 2209 | OG1 | THR | 183 | 20.203 | 77.844 | 35.121 | 1.00 | 36.22 | B |
| | ATOM | 2210 | HG1 | THR | 183 | 19.691 | 77.402 | 34.438 | 1.00 | 0.00 | B |
| | ATOM | 2211 | CG2 | THR | 183 | 22.028 | 79.347 | 35.563 | 1.00 | 20.20 | B |
| | ATOM | 2212 | C | THR | 183 | 18.936 | 79.531 | 33.646 | 1.00 | 18.10 | B |
| 15 | ATOM | 2213 | O | THR | 183 | 18.178 | 80.193 | 34.360 | 1.00 | 19.07 | B |
| | ATOM | 2214 | N | GLN | 184 | 18.509 | 78.607 | 32.797 | 1.00 | 15.96 | B |
| | ATOM | 2215 | H | GLN | 184 | 19.158 | 78.154 | 32.225 | 1.00 | 0.00 | B |
| | ATOM | 2216 | CA | GLN | 184 | 17.107 | 78.245 | 32.693 | 1.00 | 16.73 | B |
| 20 | ATOM | 2217 | CB | GLN | 184 | 16.564 | 78.600 | 31.305 | 1.00 | 20.17 | B |
| | ATOM | 2218 | CG | GLN | 184 | 16.243 | 80.079 | 31.118 | 1.00 | 15.38 | B |
| | ATOM | 2219 | CD | GLN | 184 | 15.181 | 80.307 | 30.063 | 1.00 | 14.63 | B |
| | ATOM | 2220 | OE1 | GLN | 184 | 14.165 | 80.926 | 30.326 | 1.00 | 17.14 | B |
| | ATOM | 2221 | NE2 | GLN | 184 | 15.416 | 79.801 | 28.859 | 1.00 | 17.84 | B |
| | ATOM | 2222 | HE21 | GLN | 184 | 16.245 | 79.305 | 28.694 | 1.00 | 0.00 | B |
| 25 | ATOM | 2223 | HE22 | GLN | 184 | 14.737 | 79.942 | 28.172 | 1.00 | 0.00 | B |
| | ATOM | 2224 | C | GLN | 184 | 17.023 | 76.740 | 32.905 | 1.00 | 16.49 | B |
| | ATOM | 2225 | O | GLN | 184 | 17.841 | 75.981 | 32.377 | 1.00 | 18.75 | B |
| | ATOM | 2226 | N | VAL | 185 | 16.043 | 76.311 | 33.685 | 1.00 | 19.05 | B |
| 30 | ATOM | 2227 | H | VAL | 185 | 15.437 | 76.962 | 34.095 | 1.00 | 0.00 | B |
| | ATOM | 2228 | CA | VAL | 185 | 15.849 | 74.895 | 33.943 | 1.00 | 15.68 | B |
| | ATOM | 2229 | CB | VAL | 185 | 16.145 | 74.549 | 35.437 | 1.00 | 15.74 | B |
| | ATOM | 2230 | CG1 | VAL | 185 | 15.608 | 73.149 | 35.795 | 1.00 | 14.91 | B |
| | ATOM | 2231 | CG2 | VAL | 185 | 17.641 | 74.610 | 35.686 | 1.00 | 13.27 | B |
| | ATOM | 2232 | C | VAL | 185 | 14.411 | 74.506 | 33.614 | 1.00 | 16.98 | B |
| 35 | ATOM | 2233 | O | VAL | 185 | 13.458 | 75.230 | 33.923 | 1.00 | 17.38 | B |
| | ATOM | 2234 | N | GLY | 186 | 14.296 | 73.364 | 32.948 | 1.00 | 20.72 | B |
| | ATOM | 2235 | H | GLY | 186 | 15.109 | 72.886 | 32.688 | 1.00 | 0.00 | B |
| | ATOM | 2236 | CA | GLY | 186 | 13.016 | 72.794 | 32.585 | 1.00 | 14.37 | B |
| | ATOM | 2237 | C | GLY | 186 | 13.134 | 71.359 | 33.073 | 1.00 | 16.88 | B |
| 40 | ATOM | 2238 | O | GLY | 186 | 14.252 | 70.825 | 33.165 | 1.00 | 10.74 | B |
| | ATOM | 2239 | N | ILE | 187 | 12.020 | 70.721 | 33.409 | 1.00 | 12.53 | B |
| | ATOM | 2240 | H | ILE | 187 | 11.152 | 71.172 | 33.346 | 1.00 | 0.00 | B |
| | ATOM | 2241 | CA | ILE | 187 | 12.104 | 69.344 | 33.869 | 1.00 | 14.75 | B |
| | ATOM | 2242 | CB | ILE | 187 | 11.766 | 69.193 | 35.366 | 1.00 | 9.81 | B |
| 45 | ATOM | 2243 | CG2 | ILE | 187 | 11.733 | 67.712 | 35.742 | 1.00 | 10.78 | B |
| | ATOM | 2244 | CG1 | ILE | 187 | 12.818 | 69.901 | 36.207 | 1.00 | 10.95 | B |
| | ATOM | 2245 | CD1 | ILE | 187 | 12.517 | 69.886 | 37.678 | 1.00 | 7.68 | B |
| | ATOM | 2246 | C | ILE | 187 | 11.191 | 68.422 | 33.105 | 1.00 | 12.90 | B |
| | ATOM | 2247 | O | ILE | 187 | 10.022 | 68.699 | 32.908 | 1.00 | 14.75 | B |
| 50 | ATOM | 2248 | N | VAL | 188 | 11.756 | 67.299 | 32.696 | 1.00 | 20.73 | B |
| | ATOM | 2249 | H | VAL | 188 | 12.703 | 67.157 | 32.892 | 1.00 | 0.00 | B |
| | ATOM | 2250 | CA | VAL | 188 | 11.040 | 66.267 | 31.970 | 1.00 | 18.34 | B |
| | ATOM | 2251 | CB | VAL | 188 | 11.748 | 65.977 | 30.620 | 1.00 | 23.42 | B |
| | ATOM | 2252 | CG1 | VAL | 188 | 11.363 | 64.610 | 30.107 | 1.00 | 17.83 | B |
| 55 | ATOM | 2253 | CG2 | VAL | 188 | 11.432 | 67.075 | 29.602 | 1.00 | 16.65 | B |
| | ATOM | 2254 | C | VAL | 188 | 11.077 | 64.992 | 32.831 | 1.00 | 22.16 | B |
| | ATOM | 2255 | O | VAL | 188 | 12.126 | 64.630 | 33.373 | 1.00 | 12.92 | B |
| | ATOM | 2256 | N | GLN | 189 | 9.929 | 64.338 | 33.014 | 1.00 | 19.46 | B |
| 60 | ATOM | 2257 | H | GLN | 189 | 9.092 | 64.704 | 32.661 | 1.00 | 0.00 | B |
| | ATOM | 2258 | CA | GLN | 189 | 9.938 | 63.076 | 33.742 | 1.00 | 20.85 | B |
| | ATOM | 2259 | CB | GLN | 189 | 9.039 | 63.076 | 34.980 | 1.00 | 16.60 | B |
| | ATOM | 2260 | CG | GLN | 189 | 8.890 | 61.643 | 35.564 | 1.00 | 16.53 | B |
| | ATOM | 2261 | CD | GLN | 189 | 8.284 | 61.597 | 36.966 | 1.00 | 18.48 | B |
| | ATOM | 2262 | OE1 | GLN | 189 | 8.274 | 60.553 | 37.608 | 1.00 | 17.85 | B |
| 65 | ATOM | 2263 | NE2 | GLN | 189 | 7.777 | 62.734 | 37.431 | 1.00 | 22.55 | B |
| | ATOM | 2264 | HE21 | GLN | 189 | 7.800 | 63.546 | 36.889 | 1.00 | 0.00 | B |
| | ATOM | 2265 | HE22 | GLN | 189 | 7.387 | 62.711 | 38.332 | 1.00 | 0.00 | B |
| | ATOM | 2266 | C | GLN | 189 | 9.444 | 62.015 | 32.769 | 1.00 | 18.02 | B |
| | ATOM | 2267 | O | GLN | 189 | 8.630 | 62.295 | 31.903 | 1.00 | 13.48 | B |
| 70 | ATOM | 2268 | N | TYR | 190 | 9.963 | 60.799 | 32.897 | 1.00 | 17.53 | B |
| | ATOM | 2269 | H | TYR | 190 | 10.629 | 60.631 | 33.593 | 1.00 | 0.00 | B |
| | ATOM | 2270 | CA | TYR | 190 | 9.553 | 59.725 | 32.022 | 1.00 | 16.18 | B |
| | ATOM | 2271 | CB | TYR | 190 | 10.587 | 59.512 | 30.894 | 1.00 | 21.58 | B |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| | ATOM | 2272 | CG | TYR | 190 | 11.882 | 58.859 | 31.318 | 1.00 | 24.13 | B |
| | ATOM | 2273 | CD1 | TYR | 190 | 12.035 | 57.474 | 31.253 | 1.00 | 29.37 | B |
| | ATOM | 2274 | CE1 | TYR | 190 | 13.194 | 56.859 | 31.702 | 1.00 | 26.64 | B |
| | ATOM | 2275 | CD2 | TYR | 190 | 12.937 | 59.617 | 31.835 | 1.00 | 22.88 | B |
| 5 | ATOM | 2276 | CE2 | TYR | 190 | 14.105 | 59.006 | 32.283 | 1.00 | 22.43 | B |
| | ATOM | 2277 | CZ | TYR | 190 | 14.220 | 57.632 | 32.221 | 1.00 | 24.14 | B |
| | ATOM | 2278 | OH | TYR | 190 | 15.330 | 57.013 | 32.741 | 1.00 | 25.80 | B |
| | ATOM | 2279 | HH | TYR | 190 | 15.251 | 56.064 | 32.618 | 1.00 | 0.00 | B |
| | ATOM | 2280 | C | TYR | 190 | 9.346 | 58.474 | 32.860 | 1.00 | 17.06 | B |
| 10 | ATOM | 2281 | O | TYR | 190 | 9.753 | 58.408 | 34.027 | 1.00 | 19.81 | B |
| | ATOM | 2282 | N | GLY | 191 | 8.666 | 57.502 | 32.273 | 1.00 | 18.92 | B |
| | ATOM | 2283 | H | GLY | 191 | 8.353 | 57.624 | 31.354 | 1.00 | 0.00 | B |
| | ATOM | 2284 | CA | GLY | 191 | 8.373 | 56.255 | 32.963 | 1.00 | 16.20 | B |
| | ATOM | 2285 | C | GLY | 191 | 7.278 | 55.625 | 32.137 | 1.00 | 17.90 | B |
| 15 | ATOM | 2286 | O | GLY | 191 | 6.100 | 55.732 | 32.480 | 1.00 | 34.36 | B |
| | ATOM | 2287 | N | GLU | 192 | 7.672 | 54.993 | 31.041 | 1.00 | 16.02 | B |
| | ATOM | 2288 | H | GLU | 192 | 8.631 | 54.939 | 30.847 | 1.00 | 0.00 | B |
| | ATOM | 2289 | CA | GLU | 192 | 6.728 | 54.371 | 30.100 | 1.00 | 24.28 | B |
| | ATOM | 2290 | CB | GLU | 192 | 5.433 | 53.920 | 30.798 | 1.00 | 31.95 | B |
| 20 | ATOM | 2291 | CG | GLU | 192 | 5.253 | 52.419 | 30.945 | 1.00 | 36.40 | B |
| | ATOM | 2292 | CD | GLU | 192 | 4.309 | 52.063 | 32.084 | 1.00 | 46.73 | B |
| | ATOM | 2293 | OE1 | GLU | 192 | 3.996 | 50.864 | 32.253 | 1.00 | 46.15 | B |
| | ATOM | 2294 | OE2 | GLU | 192 | 3.878 | 52.985 | 32.815 | 1.00 | 50.61 | B |
| | ATOM | 2295 | C | GLU | 192 | 6.397 | 55.450 | 29.077 | 1.00 | 19.84 | B |
| 25 | ATOM | 2296 | O | GLU | 192 | 6.518 | 55.239 | 27.870 | 1.00 | 16.66 | B |
| | ATOM | 2297 | N | ASN | 193 | 5.990 | 56.614 | 29.580 | 1.00 | 13.96 | B |
| | ATOM | 2298 | H | ASN | 193 | 5.913 | 56.713 | 30.550 | 1.00 | 0.00 | B |
| | ATOM | 2299 | CA | ASN | 193 | 5.659 | 57.750 | 28.722 | 1.00 | 18.10 | B |
| | ATOM | 2300 | CB | ASN | 193 | 4.150 | 58.065 | 28.785 | 1.00 | 17.15 | B |
| 30 | ATOM | 2301 | CG | ASN | 193 | 3.290 | 56.962 | 28.183 | 1.00 | 17.46 | B |
| | ATOM | 2302 | OD1 | ASN | 193 | 3.165 | 56.857 | 26.965 | 1.00 | 24.21 | B |
| | ATOM | 2303 | ND2 | ASN | 193 | 2.690 | 56.138 | 29.040 | 1.00 | 9.82 | B |
| | ATOM | 2304 | HD21 | ASN | 193 | 2.815 | 56.262 | 30.004 | 1.00 | 0.00 | B |
| | ATOM | 2305 | HD22 | ASN | 193 | 2.135 | 55.426 | 28.665 | 1.00 | 0.00 | B |
| 35 | ATOM | 2306 | C | ASN | 193 | 6.468 | 58.961 | 29.202 | 1.00 | 16.97 | B |
| | ATOM | 2307 | O | ASN | 193 | 7.080 | 58.918 | 30.280 | 1.00 | 19.37 | B |
| | ATOM | 2308 | N | VAL | 194 | 6.470 | 60.025 | 28.404 | 1.00 | 13.36 | B |
| | ATOM | 2309 | H | VAL | 194 | 5.964 | 59.992 | 27.567 | 1.00 | 0.00 | B |
| | ATOM | 2310 | CA | VAL | 194 | 7.204 | 61.250 | 28.734 | 1.00 | 18.46 | B |
| 40 | ATOM | 2311 | CB | VAL | 194 | 8.117 | 61.699 | 27.555 | 1.00 | 17.45 | B |
| | ATOM | 2312 | CG1 | VAL | 194 | 9.043 | 62.818 | 28.003 | 1.00 | 16.70 | B |
| | ATOM | 2313 | CG2 | VAL | 194 | 8.901 | 60.526 | 27.022 | 1.00 | 11.05 | B |
| | ATOM | 2314 | C | VAL | 194 | 6.284 | 62.417 | 29.047 | 1.00 | 18.32 | B |
| | ATOM | 2315 | O | VAL | 194 | 5.377 | 62.710 | 28.273 | 1.00 | 17.95 | B |
| 45 | ATOM | 2316 | N | THR | 195 | 6.543 | 63.095 | 30.164 | 1.00 | 18.97 | B |
| | ATOM | 2317 | H | THR | 195 | 7.285 | 62.797 | 30.728 | 1.00 | 0.00 | B |
| | ATOM | 2318 | CA | THR | 195 | 5.768 | 64.265 | 30.582 | 1.00 | 20.52 | B |
| | ATOM | 2319 | CB | THR | 195 | 5.012 | 63.982 | 31.906 | 1.00 | 18.21 | B |
| | ATOM | 2320 | OG1 | THR | 195 | 5.765 | 64.482 | 33.014 | 1.00 | 30.10 | B |
| 50 | ATOM | 2321 | HG1 | THR | 195 | 5.291 | 64.302 | 33.830 | 1.00 | 0.00 | B |
| | ATOM | 2322 | CG2 | THR | 195 | 4.828 | 62.510 | 32.091 | 1.00 | 23.60 | B |
| | ATOM | 2323 | C | THR | 195 | 6.673 | 65.486 | 30.791 | 1.00 | 24.72 | B |
| | ATOM | 2324 | O | THR | 195 | 7.792 | 65.355 | 31.302 | 1.00 | 25.20 | B |
| | ATOM | 2325 | N | HIS | 196 | 6.216 | 66.669 | 30.371 | 1.00 | 24.33 | B |
| 55 | ATOM | 2326 | H | HIS | 196 | 5.347 | 66.719 | 29.922 | 1.00 | 0.00 | B |
| | ATOM | 2327 | CA | HIS | 196 | 6.997 | 67.890 | 30.576 | 1.00 | 20.06 | B |
| | ATOM | 2328 | CB | HIS | 196 | 6.787 | 68.891 | 29.438 | 1.00 | 20.11 | B |
| | ATOM | 2329 | CG | HIS | 196 | 7.414 | 68.468 | 28.144 | 1.00 | 31.04 | B |
| | ATOM | 2330 | CD2 | HIS | 196 | 6.916 | 67.757 | 27.103 | 1.00 | 32.61 | B |
| 60 | ATOM | 2331 | ND1 | HIS | 196 | 8.723 | 68.754 | 27.823 | 1.00 | 32.93 | B |
| | ATOM | 2332 | HD1 | HIS | 196 | 9.343 | 69.258 | 28.384 | 1.00 | 0.00 | B |
| | ATOM | 2333 | CE1 | HIS | 196 | 9.008 | 68.235 | 26.640 | 1.00 | 30.15 | B |
| | ATOM | 2334 | NE2 | HIS | 196 | 7.929 | 67.625 | 26.183 | 1.00 | 29.88 | B |
| | ATOM | 2335 | HE2 | HIS | 196 | 7.865 | 67.157 | 25.331 | 1.00 | 0.00 | B |
| 65 | ATOM | 2336 | C | HIS | 196 | 6.449 | 68.473 | 31.864 | 1.00 | 23.53 | B |
| | ATOM | 2337 | O | HIS | 196 | 5.330 | 68.968 | 31.872 | 1.00 | 24.48 | B |
| | ATOM | 2338 | N | GLU | 197 | 7.214 | 68.392 | 32.959 | 1.00 | 21.43 | B |
| | ATOM | 2339 | H | GLU | 197 | 8.101 | 67.980 | 32.898 | 1.00 | 0.00 | B |
| | ATOM | 2340 | CA | GLU | 197 | 6.745 | 68.908 | 34.244 | 1.00 | 21.98 | B |
| 70 | ATOM | 2341 | CB | GLU | 197 | 7.635 | 68.416 | 35.385 | 1.00 | 22.07 | B |
| | ATOM | 2342 | CG | GLU | 197 | 7.553 | 66.900 | 35.626 | 1.00 | 22.26 | B |
| | ATOM | 2343 | CD | GLU | 197 | 6.265 | 66.461 | 36.330 | 1.00 | 19.16 | B |
| | ATOM | 2344 | OE1 | GLU | 197 | 5.436 | 67.324 | 36.655 | 1.00 | 21.45 | B |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| | ATOM | 2345 | OE2 | GLU | 197 | 6.080 | 65.252 | 36.559 | 1.00 | 25.81 | B |
| | ATOM | 2346 | C | GLU | 197 | 6.697 | 70.432 | 34.179 | 1.00 | 21.01 | B |
| | ATOM | 2347 | O | GLU | 197 | 5.771 | 71.057 | 34.704 | 1.00 | 20.20 | B |
| | ATOM | 2348 | N | PHE | 198 | 7.715 | 71.028 | 33.568 | 1.00 | 20.63 | B |
| 5 | ATOM | 2349 | H | PHE | 198 | 8.475 | 70.486 | 33.270 | 1.00 | 0.00 | B |
| | ATOM | 2350 | CA | PHE | 198 | 7.733 | 72.465 | 33.329 | 1.00 | 16.85 | B |
| | ATOM | 2351 | CB | PHE | 198 | 7.846 | 73.321 | 34.618 | 1.00 | 19.79 | B |
| | ATOM | 2352 | CG | PHE | 198 | 9.077 | 73.099 | 35.447 | 1.00 | 18.93 | B |
| | ATOM | 2353 | CD1 | PHE | 198 | 10.282 | 73.736 | 35.134 | 1.00 | 15.68 | B |
| 10 | ATOM | 2354 | CD2 | PHE | 198 | 9.003 | 72.358 | 36.619 | 1.00 | 17.58 | B |
| | ATOM | 2355 | CE1 | PHE | 198 | 11.389 | 73.642 | 35.984 | 1.00 | 8.10 | B |
| | ATOM | 2356 | CE2 | PHE | 198 | 10.113 | 72.258 | 37.480 | 1.00 | 17.77 | B |
| | ATOM | 2357 | CZ | PHE | 198 | 11.307 | 72.909 | 37.154 | 1.00 | 18.12 | B |
| | ATOM | 2358 | C | PHE | 198 | 8.773 | 72.827 | 32.285 | 1.00 | 23.38 | B |
| 15 | ATOM | 2359 | O | PHE | 198 | 9.848 | 72.210 | 32.191 | 1.00 | 19.68 | B |
| | ATOM | 2360 | N | ASN | 199 | 8.403 | 73.797 | 31.457 | 1.00 | 22.68 | B |
| | ATOM | 2361 | H | ASN | 199 | 7.536 | 74.227 | 31.581 | 1.00 | 0.00 | B |
| | ATOM | 2362 | CA | ASN | 199 | 9.251 | 74.241 | 30.379 | 1.00 | 19.07 | B |
| | ATOM | 2363 | CB | ASN | 199 | 8.402 | 74.980 | 29.342 | 1.00 | 18.17 | B |
| 20 | ATOM | 2364 | CG | ASN | 199 | 7.545 | 74.033 | 28.511 | 1.00 | 16.13 | B |
| | ATOM | 2365 | OD1 | ASN | 199 | 7.520 | 72.824 | 28.741 | 1.00 | 21.16 | B |
| | ATOM | 2366 | ND2 | ASN | 199 | 6.849 | 74.579 | 27.532 | 1.00 | 18.89 | B |
| | ATOM | 2367 | HD21 | ASN | 199 | 6.902 | 75.547 | 27.376 | 1.00 | 0.00 | B |
| | ATOM | 2368 | HD22 | ASN | 199 | 6.292 | 73.989 | 26.986 | 1.00 | 0.00 | B |
| 25 | ATOM | 2369 | C | ASN | 199 | 10.434 | 75.094 | 30.832 | 1.00 | 15.04 | B |
| | ATOM | 2370 | O | ASN | 199 | 10.465 | 75.613 | 31.944 | 1.00 | 15.97 | B |
| | ATOM | 2371 | N | LEU | 200 | 11.414 | 75.189 | 29.935 | 1.00 | 20.27 | B |
| | ATOM | 2372 | H | LEU | 200 | 11.297 | 74.727 | 29.080 | 1.00 | 0.00 | B |
| | ATOM | 2373 | CA | LEU | 200 | 12.655 | 75.939 | 30.140 | 1.00 | 20.09 | B |
| 30 | ATOM | 2374 | CB | LEU | 200 | 13.504 | 75.847 | 28.859 | 1.00 | 20.33 | B |
| | ATOM | 2375 | CG | LEU | 200 | 15.000 | 75.481 | 28.771 | 1.00 | 19.69 | B |
| | ATOM | 2376 | CD1 | LEU | 200 | 15.510 | 74.719 | 29.975 | 1.00 | 14.91 | B |
| | ATOM | 2377 | CD2 | LEU | 200 | 15.189 | 74.680 | 27.506 | 1.00 | 11.40 | B |
| | ATOM | 2378 | C | LEU | 200 | 12.387 | 77.404 | 30.468 | 1.00 | 18.48 | B |
| 35 | ATOM | 2379 | O | LEU | 200 | 13.155 | 78.034 | 31.193 | 1.00 | 20.99 | B |
| | ATOM | 2380 | N | ASN | 201 | 11.295 | 77.949 | 29.940 | 1.00 | 13.45 | B |
| | ATOM | 2381 | H | ASN | 201 | 10.701 | 77.403 | 29.382 | 1.00 | 0.00 | B |
| | ATOM | 2382 | CA | ASN | 201 | 10.978 | 79.350 | 30.190 | 1.00 | 22.91 | B |
| | ATOM | 2383 | CB | ASN | 201 | 10.645 | 80.061 | 28.877 | 1.00 | 23.93 | B |
| 40 | ATOM | 2384 | CG | ASN | 201 | 9.360 | 79.545 | 28.229 | 1.00 | 25.62 | B |
| | ATOM | 2385 | OD1 | ASN | 201 | 9.048 | 79.911 | 27.103 | 1.00 | 32.16 | B |
| | ATOM | 2386 | ND2 | ASN | 201 | 8.624 | 78.700 | 28.932 | 1.00 | 24.92 | B |
| | ATOM | 2387 | HD21 | ASN | 201 | 8.908 | 78.429 | 29.828 | 1.00 | 0.00 | B |
| | ATOM | 2388 | HD22 | ASN | 201 | 7.801 | 78.368 | 28.519 | 1.00 | 0.00 | B |
| 45 | ATOM | 2389 | C | ASN | 201 | 9.826 | 79.549 | 31.162 | 1.00 | 24.74 | B |
| | ATOM | 2390 | O | ASN | 201 | 9.352 | 80.664 | 31.329 | 1.00 | 21.95 | B |
| | ATOM | 2391 | N | LYS | 202 | 9.378 | 78.468 | 31.789 | 1.00 | 27.24 | B |
| | ATOM | 2392 | H | LYS | 202 | 9.806 | 77.604 | 31.615 | 1.00 | 0.00 | B |
| | ATOM | 2393 | CA | LYS | 202 | 8.261 | 78.527 | 32.735 | 1.00 | 28.50 | B |
| 50 | ATOM | 2394 | CB | LYS | 202 | 7.936 | 77.122 | 33.249 | 1.00 | 35.35 | B |
| | ATOM | 2395 | CG | LYS | 202 | 6.537 | 77.001 | 33.861 | 1.00 | 44.45 | B |
| | ATOM | 2396 | CD | LYS | 202 | 5.511 | 76.529 | 32.828 | 1.00 | 51.43 | B |
| | ATOM | 2397 | CE | LYS | 202 | 5.819 | 75.112 | 32.334 | 1.00 | 52.91 | B |
| | ATOM | 2398 | NZ | LYS | 202 | 5.156 | 74.748 | 31.049 | 1.00 | 49.04 | B |
| 55 | ATOM | 2399 | HZ1 | LYS | 202 | 5.462 | 75.400 | 30.301 | 1.00 | 0.00 | B |
| | ATOM | 2400 | HZ2 | LYS | 202 | 4.124 | 74.807 | 31.163 | 1.00 | 0.00 | B |
| | ATOM | 2401 | HZ3 | LYS | 202 | 5.419 | 73.774 | 30.788 | 1.00 | 0.00 | B |
| | ATOM | 2402 | C | LYS | 202 | 8.450 | 79.451 | 33.934 | 1.00 | 25.89 | B |
| | ATOM | 2403 | O | LYS | 202 | 7.550 | 80.227 | 34.260 | 1.00 | 25.05 | B |
| 60 | ATOM | 2404 | N | TYR | 203 | 9.617 | 79.348 | 34.577 | 1.00 | 22.72 | B |
| | ATOM | 2405 | H | TYR | 203 | 10.276 | 78.722 | 34.225 | 1.00 | 0.00 | B |
| | ATOM | 2406 | CA | TYR | 203 | 9.978 | 80.123 | 35.770 | 1.00 | 26.57 | B |
| | ATOM | 2407 | CB | TYR | 203 | 10.246 | 79.166 | 36.937 | 1.00 | 20.51 | B |
| | ATOM | 2408 | CG | TYR | 203 | 9.065 | 78.303 | 37.215 | 1.00 | 23.59 | B |
| 65 | ATOM | 2409 | CD1 | TYR | 203 | 9.075 | 76.941 | 36.901 | 1.00 | 24.81 | B |
| | ATOM | 2410 | CE1 | TYR | 203 | 7.927 | 76.163 | 37.057 | 1.00 | 23.81 | B |
| | ATOM | 2411 | CD2 | TYR | 203 | 7.886 | 78.870 | 37.706 | 1.00 | 26.42 | B |
| | ATOM | 2412 | CE2 | TYR | 203 | 6.741 | 78.113 | 37.871 | 1.00 | 28.83 | B |
| | ATOM | 2413 | CZ | TYR | 203 | 6.762 | 76.763 | 37.542 | 1.00 | 32.83 | B |
| 70 | ATOM | 2414 | OH | TYR | 203 | 5.598 | 76.043 | 37.683 | 1.00 | 29.24 | B |
| | ATOM | 2415 | HH | TYR | 203 | 5.758 | 75.133 | 37.423 | 1.00 | 0.00 | B |
| | ATOM | 2416 | C | TYR | 203 | 11.201 | 81.013 | 35.569 | 1.00 | 27.09 | B |
| | ATOM | 2417 | O | TYR | 203 | 12.229 | 80.563 | 35.056 | 1.00 | 24.90 | B |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 2418 | N | SER | 204 | 11.089 | 82.268 | 35.995 | 1.00 | 29.38 | B |
| | ATOM | 2419 | H | SER | 204 | 10.256 | 82.561 | 36.419 | 1.00 | 0.00 | B |
| | ATOM | 2420 | CA | SER | 204 | 12.189 | 83.216 | 35.845 | 1.00 | 29.68 | B |
| | ATOM | 2421 | CB | SER | 204 | 11.701 | 84.509 | 35.158 | 1.00 | 29.69 | B |
| | ATOM | 2422 | OG | SER | 204 | 10.458 | 84.974 | 35.668 | 1.00 | 34.41 | B |
| 10 | ATOM | 2423 | HG | SER | 204 | 9.786 | 84.301 | 35.536 | 1.00 | 0.00 | B |
| | ATOM | 2424 | C | SER | 204 | 12.917 | 83.547 | 37.150 | 1.00 | 30.79 | B |
| | ATOM | 2425 | O | SER | 204 | 13.453 | 84.642 | 37.314 | 1.00 | 31.71 | B |
| | ATOM | 2426 | N | SER | 205 | 12.934 | 82.587 | 38.074 | 1.00 | 28.19 | B |
| | ATOM | 2427 | H | SER | 205 | 12.458 | 81.749 | 37.903 | 1.00 | 0.00 | B |
| 15 | ATOM | 2428 | CA | SER | 205 | 13.642 | 82.755 | 39.334 | 1.00 | 22.80 | B |
| | ATOM | 2429 | CB | SER | 205 | 12.895 | 83.709 | 40.263 | 1.00 | 23.08 | B |
| | ATOM | 2430 | OG | SER | 205 | 11.998 | 83.004 | 41.097 | 1.00 | 23.87 | B |
| | ATOM | 2431 | HG | SER | 205 | 11.543 | 83.623 | 41.672 | 1.00 | 0.00 | B |
| | ATOM | 2432 | C | SER | 205 | 13.851 | 81.395 | 40.003 | 1.00 | 25.18 | B |
| 20 | ATOM | 2433 | O | SER | 205 | 13.079 | 80.451 | 39.794 | 1.00 | 20.34 | B |
| | ATOM | 2434 | N | THR | 206 | 14.919 | 81.307 | 40.788 | 1.00 | 23.66 | B |
| | ATOM | 2435 | H | THR | 206 | 15.486 | 82.100 | 40.902 | 1.00 | 0.00 | B |
| | ATOM | 2436 | CA | THR | 206 | 15.289 | 80.086 | 41.487 | 1.00 | 27.98 | B |
| | ATOM | 2437 | CB | THR | 206 | 16.678 | 80.229 | 42.129 | 1.00 | 26.89 | B |
| 25 | ATOM | 2438 | OG1 | THR | 206 | 17.514 | 81.019 | 41.272 | 1.00 | 29.58 | B |
| | ATOM | 2439 | HG1 | THR | 206 | 17.597 | 80.587 | 40.418 | 1.00 | 0.00 | B |
| | ATOM | 2440 | CG2 | THR | 206 | 17.319 | 78.875 | 42.330 | 1.00 | 22.76 | B |
| | ATOM | 2441 | C | THR | 206 | 14.295 | 79.661 | 42.556 | 1.00 | 29.88 | B |
| | ATOM | 2442 | O | THR | 206 | 14.057 | 78.457 | 42.730 | 1.00 | 24.79 | B |
| 30 | ATOM | 2443 | N | GLU | 207 | 13.713 | 80.626 | 43.274 | 1.00 | 29.47 | B |
| | ATOM | 2444 | H | GLU | 207 | 13.932 | 81.567 | 43.109 | 1.00 | 0.00 | B |
| | ATOM | 2445 | CA | GLU | 207 | 12.746 | 80.266 | 44.308 | 1.00 | 32.79 | B |
| | ATOM | 2446 | CB | GLU | 207 | 12.209 | 81.492 | 45.089 | 1.00 | 38.54 | B |
| | ATOM | 2447 | CG | GLU | 207 | 12.696 | 82.875 | 44.665 | 1.00 | 45.27 | B |
| 35 | ATOM | 2448 | CD | GLU | 207 | 11.738 | 84.002 | 45.104 | 1.00 | 52.80 | B |
| | ATOM | 2449 | OE1 | GLU | 207 | 11.106 | 84.632 | 44.220 | 1.00 | 49.46 | B |
| | ATOM | 2450 | OE2 | GLU | 207 | 11.618 | 84.260 | 46.330 | 1.00 | 48.25 | B |
| | ATOM | 2451 | C | GLU | 207 | 11.582 | 79.567 | 43.623 | 1.00 | 30.36 | B |
| | ATOM | 2452 | O | GLU | 207 | 11.141 | 78.499 | 44.052 | 1.00 | 29.14 | B |
| 40 | ATOM | 2453 | N | GLU | 208 | 11.108 | 80.172 | 42.538 | 1.00 | 30.06 | B |
| | ATOM | 2454 | H | GLU | 208 | 11.527 | 81.005 | 42.237 | 1.00 | 0.00 | B |
| | ATOM | 2455 | CA | GLU | 208 | 9.980 | 79.635 | 41.781 | 1.00 | 24.26 | B |
| | ATOM | 2456 | CB | GLU | 208 | 9.588 | 80.606 | 40.680 | 1.00 | 25.42 | B |
| | ATOM | 2457 | CG | GLU | 208 | 8.833 | 81.818 | 41.198 | 1.00 | 32.20 | B |
| 45 | ATOM | 2458 | CD | GLU | 208 | 8.830 | 82.953 | 40.203 | 1.00 | 37.03 | B |
| | ATOM | 2459 | OE1 | GLU | 208 | 7.763 | 83.243 | 39.623 | 1.00 | 39.29 | B |
| | ATOM | 2460 | OE2 | GLU | 208 | 9.900 | 83.551 | 40.000 | 1.00 | 39.74 | B |
| | ATOM | 2461 | C | GLU | 208 | 10.223 | 78.265 | 41.174 | 1.00 | 20.07 | B |
| | ATOM | 2462 | O | GLU | 208 | 9.308 | 77.465 | 41.049 | 1.00 | 24.58 | B |
| 50 | ATOM | 2463 | N | VAL | 209 | 11.459 | 78.000 | 40.783 | 1.00 | 17.97 | B |
| | ATOM | 2464 | H | VAL | 209 | 12.154 | 78.681 | 40.891 | 1.00 | 0.00 | B |
| | ATOM | 2465 | CA | VAL | 209 | 11.798 | 76.715 | 40.198 | 1.00 | 15.42 | B |
| | ATOM | 2466 | CB | VAL | 209 | 13.158 | 76.797 | 39.466 | 1.00 | 18.29 | B |
| | ATOM | 2467 | CG1 | VAL | 209 | 13.810 | 75.418 | 39.380 | 1.00 | 13.02 | B |
| 55 | ATOM | 2468 | CG2 | VAL | 209 | 12.946 | 77.399 | 38.087 | 1.00 | 13.44 | B |
| | ATOM | 2469 | C | VAL | 209 | 11.860 | 75.669 | 41.308 | 1.00 | 16.08 | B |
| | ATOM | 2470 | O | VAL | 209 | 11.460 | 74.521 | 41.110 | 1.00 | 17.96 | B |
| | ATOM | 2471 | N | LEU | 210 | 12.345 | 76.074 | 42.480 | 1.00 | 23.26 | B |
| | ATOM | 2472 | H | LEU | 210 | 12.643 | 77.004 | 42.575 | 1.00 | 0.00 | B |
| 60 | ATOM | 2473 | CA | LEU | 210 | 12.445 | 75.166 | 43.626 | 1.00 | 24.65 | B |
| | ATOM | 2474 | CB | LEU | 210 | 13.202 | 75.824 | 44.777 | 1.00 | 19.16 | B |
| | ATOM | 2475 | CG | LEU | 210 | 14.712 | 75.955 | 44.603 | 1.00 | 29.23 | B |
| | ATOM | 2476 | CD1 | LEU | 210 | 15.270 | 76.886 | 45.687 | 1.00 | 32.84 | B |
| | ATOM | 2477 | CD2 | LEU | 210 | 15.354 | 74.576 | 44.682 | 1.00 | 27.82 | B |
| 65 | ATOM | 2478 | C | LEU | 210 | 11.051 | 74.805 | 44.099 | 1.00 | 27.07 | B |
| | ATOM | 2479 | O | LEU | 210 | 10.790 | 73.690 | 44.555 | 1.00 | 24.27 | B |
| | ATOM | 2480 | N | VAL | 211 | 10.150 | 75.770 | 44.012 | 1.00 | 27.55 | B |
| | ATOM | 2481 | H | VAL | 211 | 10.408 | 76.654 | 43.678 | 1.00 | 0.00 | B |
| | ATOM | 2482 | CA | VAL | 211 | 8.787 | 75.518 | 44.414 | 1.00 | 24.35 | B |
| 70 | ATOM | 2483 | CB | VAL | 211 | 7.966 | 76.832 | 44.404 | 1.00 | 23.80 | B |
| | ATOM | 2484 | CG1 | VAL | 211 | 6.474 | 76.535 | 44.344 | 1.00 | 22.78 | B |
| | ATOM | 2485 | CG2 | VAL | 211 | 8.292 | 77.641 | 45.661 | 1.00 | 20.18 | B |
| | ATOM | 2486 | C | VAL | 211 | 8.176 | 74.472 | 43.472 | 1.00 | 24.70 | B |
| | ATOM | 2487 | O | VAL | 211 | 7.566 | 73.504 | 43.934 | 1.00 | 24.21 | B |
| | ATOM | 2488 | N | ALA | 212 | 8.364 | 74.643 | 42.163 | 1.00 | 24.07 | B |
| | ATOM | 2489 | H | ALA | 212 | 8.883 | 75.411 | 41.847 | 1.00 | 0.00 | B |
| | ATOM | 2490 | CA | ALA | 212 | 7.806 | 73.695 | 41.183 | 1.00 | 23.91 | B |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 2491 | CB | ALA | 212 | 8.004 | 74.221 | 39.777 | 1.00 | 20.84 | B |
| | ATOM | 2492 | C | ALA | 212 | 8.416 | 72.299 | 41.279 | 1.00 | 23.54 | B |
| | ATOM | 2493 | O | ALA | 212 | 7.709 | 71.280 | 41.195 | 1.00 | 19.74 | B |
| | ATOM | 2494 | N | ALA | 213 | 9.736 | 72.270 | 41.433 | 1.00 | 22.17 | B |
| | ATOM | 2495 | H | ALA | 213 | 10.220 | 73.119 | 41.495 | 1.00 | 0.00 | B |
| 10 | ATOM | 2496 | CA | ALA | 213 | 10.484 | 71.032 | 41.516 | 1.00 | 20.06 | B |
| | ATOM | 2497 | CB | ALA | 213 | 11.966 | 71.332 | 41.523 | 1.00 | 23.28 | B |
| | ATOM | 2498 | C | ALA | 213 | 10.096 | 70.259 | 42.763 | 1.00 | 24.35 | B |
| | ATOM | 2499 | O | ALA | 213 | 10.032 | 69.034 | 42.748 | 1.00 | 24.95 | B |
| | ATOM | 2500 | N | ASN | 214 | 9.819 | 70.969 | 43.844 | 1.00 | 24.25 | B |
| 15 | ATOM | 2501 | H | ASN | 214 | 9.875 | 71.949 | 43.812 | 1.00 | 0.00 | B |
| | ATOM | 2502 | CA | ASN | 214 | 9.434 | 70.304 | 45.086 | 1.00 | 24.82 | B |
| | ATOM | 2503 | CB | ASN | 214 | 9.604 | 71.247 | 46.273 | 1.00 | 26.46 | B |
| | ATOM | 2504 | CG | ASN | 214 | 10.981 | 71.151 | 46.882 | 1.00 | 28.78 | B |
| | ATOM | 2505 | OD1 | ASN | 214 | 11.870 | 71.958 | 46.578 | 1.00 | 23.63 | B |
| 20 | ATOM | 2506 | ND2 | ASN | 214 | 11.179 | 70.153 | 47.739 | 1.00 | 25.69 | B |
| | ATOM | 2507 | HD21 | ASN | 214 | 10.444 | 69.533 | 47.941 | 1.00 | 0.00 | B |
| | ATOM | 2508 | HD22 | ASN | 214 | 12.063 | 70.070 | 48.145 | 1.00 | 0.00 | B |
| | ATOM | 2509 | C | ASN | 214 | 8.013 | 69.755 | 45.069 | 1.00 | 24.64 | B |
| | ATOM | 2510 | O | ASN | 214 | 7.606 | 69.021 | 45.974 | 1.00 | 18.78 | B |
| 25 | ATOM | 2511 | N | LYS | 215 | 7.256 | 70.103 | 44.039 | 1.00 | 23.65 | B |
| | ATOM | 2512 | H | LYS | 215 | 7.617 | 70.696 | 43.345 | 1.00 | 0.00 | B |
| | ATOM | 2513 | CA | LYS | 215 | 5.901 | 69.609 | 43.933 | 1.00 | 26.33 | B |
| | ATOM | 2514 | CB | LYS | 215 | 4.961 | 70.746 | 43.526 | 1.00 | 22.52 | B |
| | ATOM | 2515 | CG | LYS | 215 | 4.196 | 71.337 | 44.708 | 1.00 | 28.33 | B |
| 30 | ATOM | 2516 | CD | LYS | 215 | 3.432 | 72.606 | 44.316 | 1.00 | 32.87 | B |
| | ATOM | 2517 | CE | LYS | 215 | 1.978 | 72.307 | 43.951 | 1.00 | 30.67 | B |
| | ATOM | 2518 | NZ | LYS | 215 | 1.649 | 72.846 | 42.601 | 1.00 | 35.42 | B |
| | ATOM | 2519 | HZ1 | LYS | 215 | 2.271 | 72.406 | 41.892 | 1.00 | 0.00 | B |
| | ATOM | 2520 | HZ2 | LYS | 215 | 1.791 | 73.875 | 42.596 | 1.00 | 0.00 | B |
| 35 | ATOM | 2521 | HZ3 | LYS | 215 | 0.658 | 72.630 | 42.375 | 1.00 | 0.00 | B |
| | ATOM | 2522 | C | LYS | 215 | 5.760 | 68.434 | 42.960 | 1.00 | 22.45 | B |
| | ATOM | 2523 | O | LYS | 215 | 4.662 | 67.926 | 42.764 | 1.00 | 30.36 | B |
| | ATOM | 2524 | N | ILE | 216 | 6.864 | 67.976 | 42.375 | 1.00 | 16.84 | B |
| | ATOM | 2525 | H | ILE | 216 | 7.734 | 68.373 | 42.593 | 1.00 | 0.00 | B |
| 40 | ATOM | 2526 | CA | ILE | 216 | 6.781 | 66.884 | 41.415 | 1.00 | 12.02 | B |
| | ATOM | 2527 | CB | ILE | 216 | 8.023 | 66.856 | 40.498 | 1.00 | 14.58 | B |
| | ATOM | 2528 | CG2 | ILE | 216 | 8.050 | 65.566 | 39.671 | 1.00 | 19.30 | B |
| | ATOM | 2529 | CG1 | ILE | 216 | 8.007 | 68.084 | 39.574 | 1.00 | 13.98 | B |
| | ATOM | 2530 | CD1 | ILE | 216 | 9.345 | 68.390 | 38.904 | 1.00 | 13.34 | B |
| 45 | ATOM | 2531 | C | ILE | 216 | 6.586 | 65.514 | 42.061 | 1.00 | 12.93 | B |
| | ATOM | 2532 | O | ILE | 216 | 7.311 | 65.135 | 42.980 | 1.00 | 15.03 | B |
| | ATOM | 2533 | N | GLY | 217 | 5.581 | 64.785 | 41.580 | 1.00 | 17.89 | B |
| | ATOM | 2534 | H | GLY | 217 | 5.022 | 65.150 | 40.868 | 1.00 | 0.00 | B |
| | ATOM | 2535 | CA | GLY | 217 | 5.304 | 63.452 | 42.103 | 1.00 | 17.34 | B |
| 50 | ATOM | 2536 | C | GLY | 217 | 5.749 | 62.385 | 41.112 | 1.00 | 14.75 | B |
| | ATOM | 2537 | O | GLY | 217 | 5.675 | 62.588 | 39.898 | 1.00 | 15.21 | B |
| | ATOM | 2538 | N | ARG | 218 | 6.207 | 61.248 | 41.631 | 1.00 | 14.09 | B |
| | ATOM | 2539 | H | ARG | 218 | 6.226 | 61.146 | 42.604 | 1.00 | 0.00 | B |
| | ATOM | 2540 | CA | ARG | 218 | 6.683 | 60.152 | 40.797 | 1.00 | 17.47 | B |
| 55 | ATOM | 2541 | CB | ARG | 218 | 7.195 | 59.023 | 41.707 | 1.00 | 21.57 | B |
| | ATOM | 2542 | CG | ARG | 218 | 6.442 | 57.725 | 41.637 | 1.00 | 25.79 | B |
| | ATOM | 2543 | CD | ARG | 218 | 7.384 | 56.563 | 41.388 | 1.00 | 22.17 | B |
| | ATOM | 2544 | NE | ARG | 218 | 7.509 | 55.752 | 42.588 | 1.00 | 16.26 | B |
| | ATOM | 2545 | HE | ARG | 218 | 6.793 | 55.112 | 42.782 | 1.00 | 0.00 | B |
| 60 | ATOM | 2546 | CZ | ARG | 218 | 8.531 | 55.814 | 43.431 | 1.00 | 16.32 | B |
| | ATOM | 2547 | NH1 | ARG | 218 | 9.521 | 56.644 | 43.210 | 1.00 | 28.95 | B |
| | ATOM | 2548 | HH11 | ARG | 218 | 9.511 | 57.229 | 42.399 | 1.00 | 0.00 | B |
| | ATOM | 2549 | HH12 | ARG | 218 | 10.287 | 56.689 | 43.849 | 1.00 | 0.00 | B |
| | ATOM | 2550 | NH2 | ARG | 218 | 8.546 | 55.054 | 44.512 | 1.00 | 33.70 | B |
| 65 | ATOM | 2551 | HH21 | ARG | 218 | 7.789 | 54.425 | 44.693 | 1.00 | 0.00 | B |
| | ATOM | 2552 | HH22 | ARG | 218 | 9.316 | 55.104 | 45.146 | 1.00 | 0.00 | B |
| | ATOM | 2553 | C | ARG | 218 | 5.533 | 59.701 | 39.912 | 1.00 | 14.35 | B |
| | ATOM | 2554 | O | ARG | 218 | 4.524 | 59.251 | 40.405 | 1.00 | 19.15 | B |
| | ATOM | 2555 | N | GLN | 219 | 5.670 | 59.815 | 38.597 | 1.00 | 17.48 | B |
| 70 | ATOM | 2556 | H | GLN | 219 | 6.506 | 60.148 | 38.210 | 1.00 | 0.00 | B |
| | ATOM | 2557 | CA | GLN | 219 | 4.552 | 59.438 | 37.749 | 1.00 | 26.72 | B |
| | ATOM | 2558 | CB | GLN | 219 | 4.664 | 60.107 | 36.363 | 1.00 | 23.72 | B |
| | ATOM | 2559 | CG | GLN | 219 | 5.223 | 59.280 | 35.221 | 1.00 | 25.69 | B |
| | ATOM | 2560 | CD | GLN | 219 | 5.649 | 60.171 | 34.056 | 1.00 | 33.29 | B |
| | ATOM | 2561 | OE1 | GLN | 219 | 5.982 | 61.346 | 34.257 | 1.00 | 26.70 | B |
| | ATOM | 2562 | NE2 | GLN | 219 | 5.634 | 59.627 | 32.832 | 1.00 | 18.76 | B |
| | ATOM | 2563 | HE21 | GLN | 219 | 5.360 | 58.692 | 32.720 | 1.00 | 0.00 | B |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 2564 | HE22 | GLN | 219 | 5.906 | 60.191 | 32.081 | 1.00 | 0.00 | B |
| | ATOM | 2565 | C | GLN | 219 | 4.344 | 57.935 | 37.650 | 1.00 | 26.26 | B |
| | ATOM | 2566 | O | GLN | 219 | 3.210 | 57.475 | 37.527 | 1.00 | 30.40 | B |
| | ATOM | 2567 | N | GLY | 220 | 5.419 | 57.166 | 37.745 | 1.00 | 26.30 | B |
| | ATOM | 2568 | H | GLY | 220 | 6.305 | 57.568 | 37.863 | 1.00 | 0.00 | B |
| 10 | ATOM | 2569 | CA | GLY | 220 | 5.270 | 55.728 | 37.672 | 1.00 | 30.10 | B |
| | ATOM | 2570 | C | GLY | 220 | 5.364 | 55.123 | 36.282 | 1.00 | 29.97 | B |
| | ATOM | 2571 | O | GLY | 220 | 5.002 | 55.740 | 35.277 | 1.00 | 33.59 | B |
| | ATOM | 2572 | N | GLY | 221 | 5.849 | 53.889 | 36.244 | 1.00 | 35.79 | B |
| | ATOM | 2573 | H | GLY | 221 | 6.109 | 53.453 | 37.082 | 1.00 | 0.00 | B |
| 15 | ATOM | 2574 | CA | GLY | 221 | 6.004 | 53.171 | 34.998 | 1.00 | 39.72 | B |
| | ATOM | 2575 | C | GLY | 221 | 6.406 | 51.736 | 35.283 | 1.00 | 40.82 | B |
| | ATOM | 2576 | O | GLY | 221 | 7.085 | 51.463 | 36.277 | 1.00 | 41.96 | B |
| | ATOM | 2577 | N | LEU | 222 | 5.974 | 50.822 | 34.422 | 1.00 | 37.83 | B |
| | ATOM | 2578 | H | LEU | 222 | 5.424 | 51.109 | 33.665 | 1.00 | 0.00 | B |
| 20 | ATOM | 2579 | CA | LEU | 222 | 6.288 | 49.402 | 34.564 | 1.00 | 41.13 | B |
| | ATOM | 2580 | CB | LEU | 222 | 5.102 | 48.543 | 34.103 | 1.00 | 42.69 | B |
| | ATOM | 2581 | CG | LEU | 222 | 4.467 | 47.593 | 35.126 | 1.00 | 48.06 | B |
| | ATOM | 2582 | CD1 | LEU | 222 | 4.063 | 48.361 | 36.380 | 1.00 | 47.26 | B |
| | ATOM | 2583 | CD2 | LEU | 222 | 3.259 | 46.917 | 34.509 | 1.00 | 44.76 | B |
| 25 | ATOM | 2584 | C | LEU | 222 | 7.506 | 49.093 | 33.707 | 1.00 | 39.93 | B |
| | ATOM | 2585 | O | LEU | 222 | 8.193 | 48.099 | 33.931 | 1.00 | 42.67 | B |
| | ATOM | 2586 | N | GLN | 223 | 7.755 | 49.954 | 32.723 | 1.00 | 35.86 | B |
| | ATOM | 2587 | H | GLN | 223 | 7.145 | 50.711 | 32.601 | 1.00 | 0.00 | B |
| | ATOM | 2588 | CA | GLN | 223 | 8.893 | 49.825 | 31.815 | 1.00 | 35.26 | B |
| 30 | ATOM | 2589 | CB | GLN | 223 | 8.419 | 49.479 | 30.396 | 1.00 | 37.16 | B |
| | ATOM | 2590 | CG | GLN | 223 | 6.995 | 48.952 | 30.328 | 0.01 | 41.99 | B |
| | ATOM | 2591 | CD | GLN | 223 | 6.839 | 47.821 | 29.332 | 0.01 | 44.07 | B |
| | ATOM | 2592 | OE1 | GLN | 223 | 7.368 | 46.726 | 29.528 | 0.01 | 45.41 | B |
| | ATOM | 2593 | NE2 | GLN | 223 | 6.109 | 48.080 | 28.253 | 0.01 | 44.90 | B |
| 35 | ATOM | 2594 | HE21 | GLN | 223 | 5.707 | 48.966 | 28.138 | 1.00 | 0.00 | B |
| | ATOM | 2595 | HE22 | GLN | 223 | 5.997 | 47.364 | 27.601 | 1.00 | 0.00 | B |
| | ATOM | 2596 | C | GLN | 223 | 9.642 | 51.160 | 31.799 | 1.00 | 32.91 | B |
| | ATOM | 2597 | O | GLN | 223 | 9.032 | 52.218 | 31.641 | 1.00 | 24.75 | B |
| | ATOM | 2598 | N | THR | 224 | 10.961 | 51.096 | 31.969 | 1.00 | 30.99 | B |
| 40 | ATOM | 2599 | H | THR | 224 | 11.378 | 50.218 | 32.084 | 1.00 | 0.00 | B |
| | ATOM | 2600 | CA | THR | 224 | 11.814 | 52.283 | 31.989 | 1.00 | 25.14 | B |
| | ATOM | 2601 | CB | THR | 224 | 13.016 | 52.047 | 32.891 | 1.00 | 22.33 | B |
| | ATOM | 2602 | OG1 | THR | 224 | 12.548 | 51.636 | 34.177 | 1.00 | 22.14 | B |
| | ATOM | 2603 | HG1 | THR | 224 | 12.042 | 50.826 | 34.091 | 1.00 | 0.00 | B |
| 45 | ATOM | 2604 | CG2 | THR | 224 | 13.850 | 53.315 | 33.025 | 1.00 | 16.21 | B |
| | ATOM | 2605 | C | THR | 224 | 12.295 | 52.644 | 30.590 | 1.00 | 24.48 | |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 2637 | CD2 | LEU | 228 | 9.615 | 58.114 | 23.504 | 1.00 | 38.46 | B |
| | ATOM | 2638 | C | LEU | 228 | 12.349 | 59.295 | 25.577 | 1.00 | 20.10 | B |
| | ATOM | 2639 | O | LEU | 228 | 12.252 | 60.307 | 24.894 | 1.00 | 21.88 | B |
| | ATOM | 2640 | N | GLY | 229 | 12.551 | 59.309 | 26.895 | 1.00 | 17.67 | B |
| | ATOM | 2641 | H | GLY | 229 | 12.605 | 58.462 | 27.383 | 1.00 | 0.00 | B |
| 10 | ATOM | 2642 | CA | GLY | 229 | 12.692 | 60.562 | 27.618 | 1.00 | 17.97 | B |
| | ATOM | 2643 | C | GLY | 229 | 13.757 | 61.507 | 27.070 | 1.00 | 16.62 | B |
| | ATOM | 2644 | O | GLY | 229 | 13.513 | 62.691 | 26.912 | 1.00 | 16.95 | B |
| | ATOM | 2645 | N | THR | 230 | 14.934 | 60.964 | 26.780 | 1.00 | 14.32 | B |
| | ATOM | 2646 | H | THR | 230 | 15.056 | 60.004 | 26.924 | 1.00 | 0.00 | B |
| 15 | ATOM | 2647 | CA | THR | 230 | 16.052 | 61.731 | 26.255 | 1.00 | 13.65 | B |
| | ATOM | 2648 | CB | THR | 230 | 17.311 | 60.832 | 26.166 | 1.00 | 13.38 | B |
| | ATOM | 2649 | OG1 | THR | 230 | 17.904 | 60.705 | 27.472 | 1.00 | 24.82 | B |
| | ATOM | 2650 | HG1 | THR | 230 | 18.154 | 61.573 | 27.796 | 1.00 | 0.00 | B |
| | ATOM | 2651 | CG2 | THR | 230 | 18.331 | 61.413 | 25.195 | 1.00 | 16.39 | B |
| 20 | ATOM | 2652 | C | THR | 230 | 15.722 | 62.276 | 24.865 | 1.00 | 16.56 | B |
| | ATOM | 2653 | O | THR | 230 | 15.923 | 63.452 | 24.580 | 1.00 | 14.40 | B |
| | ATOM | 2654 | N | ASP | 231 | 15.223 | 61.400 | 24.008 | 1.00 | 11.84 | B |
| | ATOM | 2655 | H | ASP | 231 | 15.086 | 60.475 | 24.300 | 1.00 | 0.00 | B |
| | ATOM | 2656 | CA | ASP | 231 | 14.874 | 61.768 | 22.658 | 1.00 | 20.60 | B |
| 25 | ATOM | 2657 | CB | ASP | 231 | 14.400 | 60.521 | 21.911 | 1.00 | 23.12 | B |
| | ATOM | 2658 | CG | ASP | 231 | 14.401 | 60.703 | 20.421 | 1.00 | 23.62 | B |
| | ATOM | 2659 | OD1 | ASP | 231 | 15.451 | 61.103 | 19.881 | 1.00 | 26.06 | B |
| | ATOM | 2660 | OD2 | ASP | 231 | 13.363 | 60.450 | 19.788 | 1.00 | 19.93 | B |
| | ATOM | 2661 | C | ASP | 231 | 13.772 | 62.832 | 22.663 | 1.00 | 21.87 | B |
| 30 | ATOM | 2662 | O | ASP | 231 | 13.800 | 63.799 | 21.898 | 1.00 | 20.06 | B |
| | ATOM | 2663 | N | THR | 232 | 12.804 | 62.637 | 23.544 | 1.00 | 22.80 | B |
| | ATOM | 2664 | H | THR | 232 | 12.854 | 61.855 | 24.132 | 1.00 | 0.00 | B |
| | ATOM | 2665 | CA | THR | 232 | 11.670 | 63.537 | 23.681 | 1.00 | 22.51 | B |
| | ATOM | 2666 | CB | THR | 232 | 10.622 | 62.891 | 24.609 | 1.00 | 16.89 | B |
| 35 | ATOM | 2667 | OG1 | THR | 232 | 10.277 | 61.607 | 24.075 | 1.00 | 21.61 | B |
| | ATOM | 2668 | HG1 | THR | 232 | 11.061 | 61.055 | 24.031 | 1.00 | 0.00 | B |
| | ATOM | 2669 | CG2 | THR | 232 | 9.372 | 63.733 | 24.706 | 1.00 | 20.59 | B |
| | ATOM | 2670 | C | THR | 232 | 12.115 | 64.903 | 24.201 | 1.00 | 25.12 | B |
| | ATOM | 2671 | O | THR | 232 | 11.601 | 65.952 | 23.782 | 1.00 | 25.24 | B |
| 40 | ATOM | 2672 | N | ALA | 233 | 13.091 | 64.882 | 25.098 | 1.00 | 21.55 | B |
| | ATOM | 2673 | H | ALA | 233 | 13.457 | 64.019 | 25.383 | 1.00 | 0.00 | B |
| | ATOM | 2674 | CA | ALA | 233 | 13.635 | 66.099 | 25.674 | 1.00 | 17.44 | B |
| | ATOM | 2675 | CB | ALA | 233 | 14.498 | 65.746 | 26.865 | 1.00 | 17.88 | B |
| | ATOM | 2676 | C | ALA | 233 | 14.453 | 66.855 | 24.624 | 1.00 | 19.30 | B |
| 45 | ATOM | 2677 | O | ALA | 233 | 14.394 | 68.075 | 24.533 | 1.00 | 18.02 | B |
| | ATOM | 2678 | N | ARG | 234 | 15.197 | 66.115 | 23.815 | 1.00 | 17.81 | B |
| | ATOM | 2679 | H | ARG | 234 | 15.196 | 65.141 | 23.918 | 1.00 | 0.00 | B |
| | ATOM | 2680 | CA | ARG | 234 | 16.008 | 66.723 | 22.774 | 1.00 | 23.98 | B |
| | ATOM | 2681 | CB | ARG | 234 | 16.857 | 65.647 | 22.087 | 1.00 | 25.23 | B |
| 50 | ATOM | 2682 | CG | ARG | 234 | 17.603 | 66.121 | 20.851 | 1.00 | 28.43 | B |
| | ATOM | 2683 | CD | ARG | 234 | 18.028 | 64.952 | 19.994 | 1.00 | 25.37 | B |
| | ATOM | 2684 | NE | ARG | 234 | 17.098 | 64.763 | 18.887 | 1.00 | 35.93 | B |
| | ATOM | 2685 | HE | ARG | 234 | 16.794 | 65.558 | 18.403 | 1.00 | 0.00 | B |
| | ATOM | 2686 | CZ | ARG | 234 | 16.642 | 63.584 | 18.494 | 1.00 | 33.70 | B |
| 55 | ATOM | 2687 | NH1 | ARG | 234 | 17.036 | 62.484 | 19.120 | 1.00 | 42.49 | B |
| | ATOM | 2688 | HH11 | ARG | 234 | 17.678 | 62.545 | 19.883 | 1.00 | 0.00 | B |
| | ATOM | 2689 | HH12 | ARG | 234 | 16.693 | 61.592 | 18.824 | 1.00 | 0.00 | B |
| | ATOM | 2690 | NH2 | ARG | 234 | 15.786 | 63.507 | 17.488 | 1.00 | 34.51 | B |
| | ATOM | 2691 | HH21 | ARG | 234 | 15.485 | 64.341 | 17.023 | 1.00 | 0.00 | B |
| 60 | ATOM | 2692 | HH22 | ARG | 234 | 15.439 | 62.618 | 17.192 | 1.00 | 0.00 | B |
| | ATOM | 2693 | C | ARG | 234 | 15.071 | 67.341 | 21.747 | 1.00 | 23.74 | B |
| | ATOM | 2694 | O | ARG | 234 | 15.212 | 68.500 | 21.327 | 1.00 | 19.58 | B |
| | ATOM | 2695 | N | LYS | 235 | 14.099 | 66.535 | 21.360 | 1.00 | 22.00 | B |
| | ATOM | 2696 | H | LYS | 235 | 14.031 | 65.650 | 21.771 | 1.00 | 0.00 | B |
| 65 | ATOM | 2697 | CA | LYS | 235 | 13.136 | 66.915 | 20.349 | 1.00 | 23.75 | B |
| | ATOM | 2698 | CB | LYS | 235 | 12.365 | 65.674 | 19.907 | 1.00 | 27.18 | B |
| | ATOM | 2699 | CG | LYS | 235 | 12.541 | 65.347 | 18.434 | 1.00 | 39.17 | B |
| | ATOM | 2700 | CD | LYS | 235 | 12.592 | 63.848 | 18.206 | 1.00 | 40.05 | B |
| | ATOM | 2701 | CE | LYS | 235 | 11.203 | 63.255 | 18.179 | 1.00 | 37.98 | B |
| 70 | ATOM | 2702 | NZ | LYS | 235 | 11.172 | 62.081 | 17.280 | 1.00 | 36.28 | B |
| | ATOM | 2703 | HZ1 | LYS | 235 | 11.846 | 61.365 | 17.624 | 1.00 | 0.00 | B |
| | ATOM | 2704 | HZ2 | LYS | 235 | 11.440 | 62.374 | 16.319 | 1.00 | 0.00 | B |
| | ATOM | 2705 | HZ3 | LYS | 235 | 10.215 | 61.679 | 17.267 | 1.00 | 0.00 | B |
| | ATOM | 2706 | C | LYS | 235 | 12.159 | 67.992 | 20.776 | 1.00 | 14.66 | B |
| | ATOM | 2707 | O | LYS | 235 | 11.854 | 68.867 | 20.003 | 1.00 | 15.35 | B |
| | ATOM | 2708 | N | GLU | 236 | 11.698 | 67.938 | 22.017 | 1.00 | 19.61 | B |
| | ATOM | 2709 | H | GLU | 236 | 12.029 | 67.243 | 22.621 | 1.00 | 0.00 | B |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 2710 | CA | GLU | 236 | 10.714 | 68.893 | 22.491 | 1.00 | 19.56 | B |
| | ATOM | 2711 | CB | GLU | 236 | 9.467 | 68.131 | 22.980 | 1.00 | 17.41 | B |
| | ATOM | 2712 | CG | GLU | 236 | 8.705 | 67.442 | 21.848 | 1.00 | 12.51 | B |
| | ATOM | 2713 | CD | GLU | 236 | 7.734 | 66.365 | 22.326 | 1.00 | 20.23 | B |
| | ATOM | 2714 | OE1 | GLU | 236 | 7.147 | 66.493 | 23.416 | 1.00 | 16.25 | B |
| 10 | ATOM | 2715 | OE2 | GLU | 236 | 7.553 | 65.382 | 21.594 | 1.00 | 32.75 | B |
| | ATOM | 2716 | C | GLU | 236 | 11.134 | 69.905 | 23.552 | 1.00 | 19.85 | B |
| | ATOM | 2717 | O | GLU | 236 | 10.740 | 71.074 | 23.477 | 1.00 | 22.57 | B |
| | ATOM | 2718 | N | ALA | 237 | 11.923 | 69.477 | 24.530 | 1.00 | 13.82 | B |
| | ATOM | 2719 | H | ALA | 237 | 12.243 | 68.552 | 24.528 | 1.00 | 0.00 | B |
| 15 | ATOM | 2720 | CA | ALA | 237 | 12.320 | 70.380 | 25.609 | 1.00 | 15.91 | B |
| | ATOM | 2721 | CB | ALA | 237 | 13.031 | 69.599 | 26.715 | 1.00 | 12.47 | B |
| | ATOM | 2722 | C | ALA | 237 | 13.183 | 71.568 | 25.185 | 1.00 | 18.22 | B |
| | ATOM | 2723 | O | ALA | 237 | 13.067 | 72.647 | 25.754 | 1.00 | 20.95 | B |
| | ATOM | 2724 | N | PHE | 238 | 14.050 | 71.372 | 24.202 | 1.00 | 20.05 | B |
| 20 | ATOM | 2725 | H | PHE | 238 | 14.094 | 70.495 | 23.767 | 1.00 | 0.00 | B |
| | ATOM | 2726 | CA | PHE | 238 | 14.938 | 72.443 | 23.757 | 1.00 | 25.75 | B |
| | ATOM | 2727 | CB | PHE | 238 | 16.286 | 71.864 | 23.411 | 1.00 | 21.10 | B |
| | ATOM | 2728 | CG | PHE | 238 | 17.058 | 71.430 | 24.607 | 1.00 | 20.59 | B |
| | ATOM | 2729 | CD1 | PHE | 238 | 17.153 | 70.081 | 24.926 | 1.00 | 10.70 | B |
| 25 | ATOM | 2730 | CD2 | PHE | 238 | 17.690 | 72.378 | 25.425 | 1.00 | 17.21 | B |
| | ATOM | 2731 | CE1 | PHE | 238 | 17.865 | 69.668 | 26.043 | 1.00 | 6.53 | B |
| | ATOM | 2732 | CE2 | PHE | 238 | 18.407 | 71.981 | 26.548 | 1.00 | 9.67 | B |
| | ATOM | 2733 | CZ | PHE | 238 | 18.498 | 70.623 | 26.860 | 1.00 | 14.30 | B |
| | ATOM | 2734 | C | PHE | 238 | 14.364 | 73.171 | 22.570 | 1.00 | 32.55 | B |
| 30 | ATOM | 2735 | O | PHE | 238 | 15.050 | 73.472 | 21.591 | 1.00 | 34.64 | B |
| | ATOM | 2736 | N | THR | 239 | 13.080 | 73.446 | 22.682 | 1.00 | 33.09 | B |
| | ATOM | 2737 | H | THR | 239 | 12.608 | 73.176 | 23.499 | 1.00 | 0.00 | B |
| | ATOM | 2738 | CA | THR | 239 | 12.344 | 74.125 | 21.651 | 1.00 | 37.89 | B |
| | ATOM | 2739 | CB | THR | 239 | 10.911 | 73.562 | 21.597 | 1.00 | 34.14 | B |
| 35 | ATOM | 2740 | OG1 | THR | 239 | 10.907 | 72.378 | 20.797 | 1.00 | 44.61 | B |
| | ATOM | 2741 | HG1 | THR | 239 | 10.019 | 72.020 | 20.758 | 1.00 | 0.00 | B |
| | ATOM | 2742 | CG2 | THR | 239 | 9.953 | 74.558 | 21.010 | 1.00 | 42.52 | B |
| | ATOM | 2743 | C | THR | 239 | 12.329 | 75.606 | 21.986 | 1.00 | 38.96 | B |
| | ATOM | 2744 | O | THR | 239 | 12.421 | 75.989 | 23.156 | 1.00 | 40.40 | B |
| 40 | ATOM | 2745 | N | GLU | 240 | 12.229 | 76.438 | 20.962 | 1.00 | 36.75 | B |
| | ATOM | 2746 | H | GLU | 240 | 12.181 | 76.087 | 20.049 | 1.00 | 0.00 | B |
| | ATOM | 2747 | CA | GLU | 240 | 12.191 | 77.867 | 21.185 | 1.00 | 42.75 | B |
| | ATOM | 2748 | CB | GLU | 240 | 12.344 | 78.604 | 19.855 | 1.00 | 50.61 | B |
| | ATOM | 2749 | CG | GLU | 240 | 11.038 | 78.872 | 19.148 | 1.00 | 62.98 | B |
| 45 | ATOM | 2750 | CD | GLU | 240 | 10.313 | 80.068 | 19.724 | 1.00 | 67.81 | B |
| | ATOM | 2751 | OE1 | GLU | 240 | 10.925 | 81.156 | 19.774 | 1.00 | 70.98 | B |
| | ATOM | 2752 | OE2 | GLU | 240 | 9.140 | 79.916 | 20.131 | 1.00 | 69.99 | B |
| | ATOM | 2753 | C | GLU | 240 | 10.843 | 78.178 | 21.843 | 1.00 | 40.19 | B |
| | ATOM | 2754 | O | GLU | 240 | 10.751 | 79.041 | 22.707 | 1.00 | 33.66 | B |
| 50 | ATOM | 2755 | N | ALA | 241 | 9.804 | 77.458 | 21.423 | 1.00 | 33.98 | B |
| | ATOM | 2756 | H | ALA | 241 | 9.936 | 76.796 | 20.714 | 1.00 | 0.00 | B |
| | ATOM | 2757 | CA | ALA | 241 | 8.471 | 77.636 | 21.986 | 1.00 | 29.60 | B |
| | ATOM | 2758 | CB | ALA | 241 | 7.492 | 76.687 | 21.316 | 1.00 | 37.19 | B |
| | ATOM | 2759 | C | ALA | 241 | 8.499 | 77.375 | 23.491 | 1.00 | 29.07 | B |
| 55 | ATOM | 2760 | O | ALA | 241 | 7.801 | 78.047 | 24.251 | 1.00 | 32.90 | B |
| | ATOM | 2761 | N | ARG | 242 | 9.312 | 76.406 | 23.916 | 1.00 | 25.07 | B |
| | ATOM | 2762 | H | ARG | 242 | 9.845 | 75.913 | 23.257 | 1.00 | 0.00 | B |
| | ATOM | 2763 | CA | ARG | 242 | 9.429 | 76.057 | 25.332 | 1.00 | 21.30 | B |
| | ATOM | 2764 | CB | ARG | 242 | 9.644 | 74.551 | 25.495 | 1.00 | 21.86 | B |
| 60 | ATOM | 2765 | CG | ARG | 242 | 8.486 | 73.680 | 24.980 | 1.00 | 18.40 | B |
| | ATOM | 2766 | CD | ARG | 242 | 8.520 | 72.317 | 25.663 | 1.00 | 23.54 | B |
| | ATOM | 2767 | NE | ARG | 242 | 7.674 | 71.334 | 25.001 | 1.00 | 27.29 | B |
| | ATOM | 2768 | HE | ARG | 242 | 7.958 | 70.990 | 24.131 | 1.00 | 0.00 | B |
| | ATOM | 2769 | CZ | ARG | 242 | 6.536 | 70.870 | 25.509 | 1.00 | 21.77 | B |
| 65 | ATOM | 2770 | NH1 | ARG | 242 | 6.106 | 71.302 | 26.686 | 1.00 | 28.61 | B |
| | ATOM | 2771 | HH11 | ARG | 242 | 6.637 | 71.979 | 27.196 | 1.00 | 0.00 | B |
| | ATOM | 2772 | HH12 | ARG | 242 | 5.249 | 70.952 | 27.064 | 1.00 | 0.00 | B |
| | ATOM | 2773 | NH2 | ARG | 242 | 5.842 | 69.967 | 24.851 | 1.00 | 21.18 | B |
| | ATOM | 2774 | HH21 | ARG | 242 | 6.171 | 69.625 | 23.969 | 1.00 | 0.00 | B |
| 70 | ATOM | 2775 | HH22 | ARG | 242 | 4.986 | 69.618 | 25.232 | 1.00 | 0.00 | B |
| | ATOM | 2776 | C | ARG | 242 | 10.538 | 76.806 | 26.071 | 1.00 | 17.43 | B |
| | ATOM | 2777 | O | ARG | 242 | 10.884 | 76.462 | 27.206 | 1.00 | 14.43 | B |
| | ATOM | 2778 | N | GLY | 243 | 11.127 | 77.800 | 25.419 | 1.00 | 15.32 | B |
| | ATOM | 2779 | H | GLY | 243 | 10.878 | 78.002 | 24.495 | 1.00 | 0.00 | B |
| 70 | ATOM | 2780 | CA | GLY | 243 | 12.146 | 78.595 | 26.096 | 1.00 | 16.02 | B |
| | ATOM | 2781 | C | GLY | 243 | 13.628 | 78.505 | 25.786 | 1.00 | 10.54 | B |
| | ATOM | 2782 | O | GLY | 243 | 14.406 | 79.182 | 26.444 | 1.00 | 20.03 | B |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 2783 | N | ALA | 244 | 14.038 | 77.716 | 24.801 | 1.00 | 10.60 | B |
| | ATOM | 2784 | H | ALA | 244 | 13.378 | 77.200 | 24.293 | 1.00 | 0.00 | B |
| | ATOM | 2785 | CA | ALA | 244 | 15.453 | 77.610 | 24.476 | 1.00 | 10.63 | B |
| | ATOM | 2786 | CB | ALA | 244 | 15.692 | 76.439 | 23.533 | 1.00 | 12.74 | B |
| | ATOM | 2787 | C | ALA | 244 | 15.916 | 78.907 | 23.828 | 1.00 | 19.09 | B |
| 10 | ATOM | 2788 | O | ALA | 244 | 15.394 | 79.329 | 22.800 | 1.00 | 22.97 | B |
| | ATOM | 2789 | N | ARG | 245 | 16.911 | 79.540 | 24.433 | 1.00 | 21.88 | B |
| | ATOM | 2790 | H | ARG | 245 | 17.308 | 79.140 | 25.235 | 1.00 | 0.00 | B |
| | ATOM | 2791 | CA | ARG | 245 | 17.429 | 80.809 | 23.942 | 1.00 | 16.43 | B |
| | ATOM | 2792 | CB | ARG | 245 | 18.037 | 81.552 | 25.122 | 1.00 | 16.53 | B |
| 15 | ATOM | 2793 | CG | ARG | 245 | 17.062 | 81.593 | 26.288 | 1.00 | 18.89 | B |
| | ATOM | 2794 | CD | ARG | 245 | 17.668 | 82.162 | 27.546 | 1.00 | 20.31 | B |
| | ATOM | 2795 | NE | ARG | 245 | 18.429 | 81.148 | 28.265 | 1.00 | 12.05 | B |
| | ATOM | 2796 | HE | ARG | 245 | 18.290 | 80.209 | 28.024 | 1.00 | 0.00 | B |
| | ATOM | 2797 | CZ | ARG | 245 | 19.290 | 81.427 | 29.230 | 1.00 | 16.66 | B |
| 20 | ATOM | 2798 | NH1 | ARG | 245 | 19.494 | 82.692 | 29.589 | 1.00 | 11.02 | B |
| | ATOM | 2799 | HH11 | ARG | 245 | 18.992 | 83.428 | 29.138 | 1.00 | 0.00 | B |
| | ATOM | 2800 | HH12 | ARG | 245 | 20.147 | 82.907 | 30.317 | 1.00 | 0.00 | B |
| | ATOM | 2801 | NH2 | ARG | 245 | 19.949 | 80.444 | 29.830 | 1.00 | 17.95 | B |
| | ATOM | 2802 | HH21 | ARG | 245 | 19.789 | 79.495 | 29.554 | 1.00 | 0.00 | B |
| 25 | ATOM | 2803 | HH22 | ARG | 245 | 20.604 | 80.649 | 30.554 | 1.00 | 0.00 | B |
| | ATOM | 2804 | C | ARG | 245 | 18.411 | 80.701 | 22.784 | 1.00 | 13.58 | B |
| | ATOM | 2805 | O | ARG | 245 | 19.106 | 79.699 | 22.632 | 1.00 | 14.35 | B |
| | ATOM | 2806 | N | ARG | 246 | 18.450 | 81.739 | 21.952 | 1.00 | 16.40 | B |
| | ATOM | 2807 | H | ARG | 246 | 17.864 | 82.504 | 22.119 | 1.00 | 0.00 | B |
| 30 | ATOM | 2808 | CA | ARG | 246 | 19.341 | 81.766 | 20.794 | 1.00 | 16.73 | B |
| | ATOM | 2809 | CB | ARG | 246 | 19.116 | 83.052 | 19.978 | 1.00 | 20.99 | B |
| | ATOM | 2810 | CG | ARG | 246 | 19.775 | 83.037 | 18.582 | 1.00 | 27.27 | B |
| | ATOM | 2811 | CD | ARG | 246 | 19.881 | 81.606 | 18.080 | 1.00 | 29.21 | B |
| | ATOM | 2812 | NE | ARG | 246 | 20.716 | 81.432 | 16.898 | 1.00 | 40.75 | B |
| 35 | ATOM | 2813 | HE | ARG | 246 | 21.467 | 80.808 | 16.959 | 1.00 | 0.00 | B |
| | ATOM | 2814 | CZ | ARG | 246 | 20.516 | 82.047 | 15.737 | 1.00 | 40.49 | B |
| | ATOM | 2815 | NH1 | ARG | 246 | 19.502 | 82.893 | 15.590 | 1.00 | 44.89 | B |
| | ATOM | 2816 | HH11 | ARG | 246 | 18.867 | 83.049 | 16.346 | 1.00 | 0.00 | B |
| | ATOM | 2817 | HH12 | ARG | 246 | 19.361 | 83.355 | 14.715 | 1.00 | 0.00 | B |
| 40 | ATOM | 2818 | NH2 | ARG | 246 | 21.323 | 81.797 | 14.715 | 1.00 | 40.11 | B |
| | ATOM | 2819 | HH21 | ARG | 246 | 22.065 | 81.130 | 14.816 | 1.00 | 0.00 | B |
| | ATOM | 2820 | HH22 | ARG | 246 | 21.185 | 82.260 | 13.841 | 1.00 | 0.00 | B |
| | ATOM | 2821 | C | ARG | 246 | 20.830 | 81.662 | 21.175 | 1.00 | 19.16 | B |
| | ATOM | 2822 | O | ARG | 246 | 21.347 | 82.479 | 21.929 | 1.00 | 19.43 | B |
| 45 | ATOM | 2823 | N | GLY | 247 | 21.505 | 80.652 | 20.651 | 1.00 | 15.61 | B |
| | ATOM | 2824 | H | GLY | 247 | 21.040 | 80.009 | 20.075 | 1.00 | 0.00 | B |
| | ATOM | 2825 | CA | GLY | 247 | 22.920 | 80.479 | 20.917 | 1.00 | 19.07 | B |
| | ATOM | 2826 | C | GLY | 247 | 23.301 | 80.022 | 22.315 | 1.00 | 19.74 | B |
| | ATOM | 2827 | O | GLY | 247 | 24.479 | 79.869 | 22.618 | 1.00 | 24.75 | B |
| 50 | ATOM | 2828 | N | VAL | 248 | 22.320 | 79.793 | 23.170 | 1.00 | 18.96 | B |
| | ATOM | 2829 | H | VAL | 248 | 21.390 | 79.916 | 22.891 | 1.00 | 0.00 | B |
| | ATOM | 2830 | CA | VAL | 248 | 22.619 | 79.361 | 24.528 | 1.00 | 16.15 | B |
| | ATOM | 2831 | CB | VAL | 248 | 21.466 | 79.725 | 25.475 | 1.00 | 11.70 | B |
| | ATOM | 2832 | CG1 | VAL | 248 | 21.742 | 79.172 | 26.871 | 1.00 | 8.03 | B |
| 55 | ATOM | 2833 | CG2 | VAL | 248 | 21.285 | 81.254 | 25.517 | 1.00 | 12.88 | B |
| | ATOM | 2834 | C | VAL | 248 | 22.851 | 77.852 | 24.542 | 1.00 | 19.75 | B |
| | ATOM | 2835 | O | VAL | 248 | 22.051 | 77.104 | 24.008 | 1.00 | 20.58 | B |
| | ATOM | 2836 | N | LYS | 249 | 23.946 | 77.410 | 25.153 | 1.00 | 21.97 | B |
| | ATOM | 2837 | H | LYS | 249 | 24.551 | 78.054 | 25.574 | 1.00 | 0.00 | B |
| 60 | ATOM | 2838 | CA | LYS | 249 | 24.269 | 75.983 | 25.204 | 1.00 | 24.74 | B |
| | ATOM | 2839 | CB | LYS | 249 | 25.668 | 75.769 | 25.795 | 1.00 | 28.79 | B |
| | ATOM | 2840 | CG | LYS | 249 | 26.782 | 75.746 | 24.731 | 1.00 | 39.64 | B |
| | ATOM | 2841 | CD | LYS | 249 | 26.332 | 76.365 | 23.395 | 1.00 | 40.06 | B |
| | ATOM | 2842 | CE | LYS | 249 | 27.485 | 76.507 | 22.393 | 1.00 | 46.49 | B |
| 65 | ATOM | 2843 | NZ | LYS | 249 | 28.289 | 77.759 | 22.567 | 1.00 | 42.34 | B |
| | ATOM | 2844 | HZ1 | LYS | 249 | 28.706 | 77.775 | 23.518 | 1.00 | 0.00 | B |
| | ATOM | 2845 | HZ2 | LYS | 249 | 27.672 | 78.587 | 22.444 | 1.00 | 0.00 | B |
| | ATOM | 2846 | HZ3 | LYS | 249 | 29.047 | 77.784 | 21.855 | 1.00 | 0.00 | B |
| | ATOM | 2847 | C | LYS | 249 | 23.268 | 75.105 | 25.945 | 1.00 | 18.56 | B |
| 70 | ATOM | 2848 | O | LYS | 249 | 22.753 | 75.467 | 27.007 | 1.00 | 15.02 | B |
| | ATOM | 2849 | N | LYS | 250 | 23.030 | 73.937 | 25.359 | 1.00 | 19.31 | B |
| | ATOM | 2850 | H | LYS | 250 | 23.514 | 73.734 | 24.531 | 1.00 | 0.00 | B |
| | ATOM | 2851 | CA | LYS | 250 | 22.101 | 72.943 | 25.864 | 1.00 | 21.51 | B |
| | ATOM | 2852 | CB | LYS | 250 | 21.440 | 72.228 | 24.684 | 1.00 | 21.98 | B |
| | ATOM | 2853 | CG | LYS | 250 | 20.819 | 73.146 | 23.641 | 1.00 | 24.29 | B |
| | ATOM | 2854 | CD | LYS | 250 | 20.380 | 72.344 | 22.404 | 1.00 | 20.75 | B |
| | ATOM | 2855 | CE | LYS | 250 | 19.318 | 73.084 | 21.606 | 1.00 | 30.12 | B |

| | | | | | | | | | | | |
|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 2856 | NZ | LYS | 250 | 19.629 | 73.074 | 20.143 | 1.00 | 33.42 | B |
| | ATOM | 2857 | HZ1 | LYS | 250 | 19.675 | 72.092 | 19.805 | 1.00 | 0.00 | B |
| | ATOM | 2858 | HZ2 | LYS | 250 | 20.546 | 73.539 | 19.983 | 1.00 | 0.00 | B |
| | ATOM | 2859 | HZ3 | LYS | 250 | 18.887 | 73.586 | 19.627 | 1.00 | 0.00 | B |
| | ATOM | 2860 | C | LYS | 250 | 22.735 | 71.894 | 26.776 | 1.00 | 23.57 | B |
| 10 | ATOM | 2861 | O | LYS | 250 | 23.707 | 71.221 | 26.394 | 1.00 | 20.92 | B |
| | ATOM | 2862 | N | VAL | 251 | 22.198 | 71.756 | 27.986 | 1.00 | 17.38 | B |
| | ATOM | 2863 | H | VAL | 251 | 21.459 | 72.339 | 28.260 | 1.00 | 0.00 | B |
| | ATOM | 2864 | CA | VAL | 251 | 22.708 | 70.748 | 28.899 | 1.00 | 17.18 | B |
| | ATOM | 2865 | CB | VAL | 251 | 23.364 | 71.338 | 30.175 | 1.00 | 11.43 | B |
| 15 | ATOM | 2866 | CG1 | VAL | 251 | 23.853 | 70.213 | 31.024 | 1.00 | 6.20 | B |
| | ATOM | 2867 | CG2 | VAL | 251 | 24.542 | 72.269 | 29.823 | 1.00 | 18.54 | B |
| | ATOM | 2868 | C | VAL | 251 | 21.573 | 69.834 | 29.354 | 1.00 | 20.95 | B |
| | ATOM | 2869 | O | VAL | 251 | 20.496 | 70.283 | 29.712 | 1.00 | 17.19 | B |
| | ATOM | 2870 | N | MET | 252 | 21.831 | 68.537 | 29.332 | 1.00 | 17.99 | B |
| 20 | ATOM | 2871 | H | MET | 252 | 22.706 | 68.228 | 29.021 | 1.00 | 0.00 | B |
| | ATOM | 2872 | CA | MET | 252 | 20.851 | 67.573 | 29.762 | 1.00 | 18.29 | B |
| | ATOM | 2873 | CB | MET | 252 | 20.513 | 66.658 | 28.570 | 1.00 | 17.87 | B |
| | ATOM | 2874 | CG | MET | 252 | 19.355 | 65.715 | 28.776 | 1.00 | 17.10 | B |
| | ATOM | 2875 | SD | MET | 252 | 19.057 | 64.546 | 27.405 | 1.00 | 35.69 | B |
| 25 | ATOM | 2876 | CE | MET | 252 | 18.612 | 65.592 | 26.112 | 1.00 | 19.60 | B |
| | ATOM | 2877 | C | MET | 252 | 21.451 | 66.778 | 30.932 | 1.00 | 15.72 | B |
| | ATOM | 2878 | O | MET | 252 | 22.568 | 66.280 | 30.827 | 1.00 | 19.38 | B |
| | ATOM | 2879 | N | VAL | 253 | 20.731 | 66.696 | 32.048 | 1.00 | 18.09 | B |
| | ATOM | 2880 | H | VAL | 253 | 19.881 | 67.176 | 32.096 | 1.00 | 0.00 | B |
| 30 | ATOM | 2881 | CA | VAL | 253 | 21.165 | 65.916 | 33.208 | 1.00 | 17.72 | B |
| | ATOM | 2882 | CB | VAL | 253 | 21.201 | 66.788 | 34.496 | 1.00 | 16.44 | B |
| | ATOM | 2883 | CG1 | VAL | 253 | 22.061 | 68.051 | 34.263 | 1.00 | 9.88 | B |
| | ATOM | 2884 | CG2 | VAL | 253 | 19.802 | 67.226 | 34.861 | 1.00 | 28.03 | B |
| | ATOM | 2885 | C | VAL | 253 | 20.151 | 64.756 | 33.379 | 1.00 | 20.14 | B |
| 35 | ATOM | 2886 | O | VAL | 253 | 18.974 | 64.981 | 33.648 | 1.00 | 18.38 | B |
| | ATOM | 2887 | N | ILE | 254 | 20.607 | 63.517 | 33.226 | 1.00 | 24.01 | B |
| | ATOM | 2888 | H | ILE | 254 | 21.557 | 63.374 | 33.037 | 1.00 | 0.00 | B |
| | ATOM | 2889 | CA | ILE | 254 | 19.715 | 62.360 | 33.335 | 1.00 | 20.30 | B |
| | ATOM | 2890 | CB | ILE | 254 | 19.903 | 61.386 | 32.137 | 1.00 | 24.38 | B |
| 40 | ATOM | 2891 | CG2 | ILE | 254 | 18.849 | 60.290 | 32.183 | 1.00 | 21.87 | B |
| | ATOM | 2892 | CG1 | ILE | 254 | 19.784 | 62.147 | 30.816 | 1.00 | 20.74 | B |
| | ATOM | 2893 | CD1 | ILE | 254 | 21.107 | 62.500 | 30.176 | 1.00 | 26.33 | B |
| | ATOM | 2894 | C | ILE | 254 | 19.911 | 61.596 | 34.635 | 1.00 | 21.12 | B |
| | ATOM | 2895 | O | ILE | 254 | 21.031 | 61.215 | 34.976 | 1.00 | 18.90 | B |
| 45 | ATOM | 2896 | N | VAL | 255 | 18.804 | 61.377 | 35.348 | 1.00 | 16.92 | B |
| | ATOM | 2897 | H | VAL | 255 | 17.951 | 61.700 | 34.986 | 1.00 | 0.00 | B |
| | ATOM | 2898 | CA | VAL | 255 | 18.796 | 60.692 | 36.629 | 1.00 | 16.15 | B |
| | ATOM | 2899 | CB | VAL | 255 | 18.178 | 61.580 | 37.725 | 1.00 | 18.84 | B |
| | ATOM | 2900 | CG1 | VAL | 255 | 18.215 | 60.856 | 39.071 | 1.00 | 10.30 | B |
| 50 | ATOM | 2901 | CG2 | VAL | 255 | 18.931 | 62.925 | 37.796 | 1.00 | 16.06 | B |
| | ATOM | 2902 | C | VAL | 255 | 17.970 | 59.434 | 36.484 | 1.00 | 13.71 | B |
| | ATOM | 2903 | O | VAL | 255 | 16.799 | 59.480 | 36.109 | 1.00 | 16.40 | B |
| | ATOM | 2904 | N | THR | 256 | 18.584 | 58.301 | 36.781 | 1.00 | 14.62 | B |
| | ATOM | 2905 | H | THR | 256 | 19.507 | 58.326 | 37.105 | 1.00 | 0.00 | B |
| 55 | ATOM | 2906 | CA | THR | 256 | 17.906 | 57.022 | 36.634 | 1.00 | 15.00 | B |
| | ATOM | 2907 | CB | THR | 256 | 17.950 | 56.564 | 35.161 | 1.00 | 17.78 | B |
| | ATOM | 2908 | OG1 | THR | 256 | 17.186 | 55.359 | 35.006 | 1.00 | 23.15 | B |
| | ATOM | 2909 | HG1 | THR | 256 | 16.277 | 55.527 | 35.259 | 1.00 | 0.00 | B |
| | ATOM | 2910 | CG2 | THR | 256 | 19.414 | 56.327 | 34.704 | 1.00 | 10.75 | B |
| 60 | ATOM | 2911 | C | THR | 256 | 18.542 | 55.954 | 37.523 | 1.00 | 16.31 | B |
| | ATOM | 2912 | O | THR | 256 | 19.740 | 56.041 | 37.862 | 1.00 | 16.43 | B |
| | ATOM | 2913 | N | ASP | 257 | 17.739 | 54.948 | 37.881 | 1.00 | 15.42 | B |
| | ATOM | 2914 | H | ASP | 257 | 16.815 | 54.937 | 37.553 | 1.00 | 0.00 | B |
| | ATOM | 2915 | CA | ASP | 257 | 18.198 | 53.872 | 38.745 | 1.00 | 15.12 | B |
| 65 | ATOM | 2916 | CB | ASP | 257 | 17.481 | 53.974 | 40.119 | 1.00 | 17.76 | B |
| | ATOM | 2917 | CG | ASP | 257 | 16.155 | 53.241 | 40.153 | 1.00 | 16.63 | B |
| | ATOM | 2918 | OD1 | ASP | 257 | 15.782 | 52.706 | 41.219 | 1.00 | 16.55 | B |
| | ATOM | 2919 | OD2 | ASP | 257 | 15.492 | 53.197 | 39.107 | 1.00 | 18.63 | B |
| | ATOM | 2920 | C | ASP | 257 | 18.067 | 52.456 | 38.158 | 1.00 | 15.10 | B |
| 70 | ATOM | 2921 | O | ASP | 257 | 17.872 | 51.478 | 38.892 | 1.00 | 17.29 | B |
| | ATOM | 2922 | N | GLY | 258 | 18.177 | 52.337 | 36.839 | 1.00 | 9.50 | B |
| | ATOM | 2923 | H | GLY | 258 | 18.302 | 53.127 | 36.277 | 1.00 | 0.00 | B |
| | ATOM | 2924 | CA | GLY | 258 | 18.108 | 51.013 | 36.240 | 1.00 | 11.28 | B |
| | ATOM | 2925 | C | GLY | 258 | 18.275 | 50.992 | 34.737 | 1.00 | 13.51 | B |
| | ATOM | 2926 | O | GLY | 258 | 18.350 | 52.038 | 34.108 | 1.00 | 17.36 | B |
| | ATOM | 2927 | N | GLU | 259 | 18.328 | 49.792 | 34.159 | 1.00 | 16.87 | B |
| | ATOM | 2928 | H | GLU | 259 | 18.257 | 48.995 | 34.723 | 1.00 | 0.00 | B |

| | | | | | | | | | | | |
|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 2929 | CA | GLU | 259 | 18.488 | 49.628 | 32.718 | 1.00 | 20.62 | B |
| | ATOM | 2930 | CB | GLU | 259 | 18.730 | 48.158 | 32.358 | 1.00 | 23.36 | B |
| | ATOM | 2931 | CG | GLU | 259 | 20.115 | 47.652 | 32.667 | 1.00 | 32.72 | B |
| | ATOM | 2932 | CD | GLU | 259 | 20.119 | 46.175 | 33.015 | 1.00 | 31.78 | B |
| | ATOM | 2933 | OE1 | GLU | 259 | 19.803 | 45.356 | 32.120 | 1.00 | 30.21 | B |
| 10 | ATOM | 2934 | OE2 | GLU | 259 | 20.441 | 45.844 | 34.178 | 1.00 | 27.13 | B |
| | ATOM | 2935 | C | GLU | 259 | 17.238 | 50.083 | 32.003 | 1.00 | 22.02 | B |
| | ATOM | 2936 | O | GLU | 259 | 16.141 | 50.060 | 32.571 | 1.00 | 22.92 | B |
| | ATOM | 2937 | N | SER | 260 | 17.383 | 50.452 | 30.736 | 1.00 | 17.73 | B |
| | ATOM | 2938 | H | SER | 260 | 18.264 | 50.419 | 30.314 | 1.00 | 0.00 | B |
| 15 | ATOM | 2939 | CA | SER | 260 | 16.226 | 50.900 | 29.987 | 1.00 | 21.31 | B |
| | ATOM | 2940 | CB | SER | 260 | 16.609 | 52.107 | 29.133 | 1.00 | 18.50 | B |
| | ATOM | 2941 | OG | SER | 260 | 17.456 | 51.716 | 28.080 | 1.00 | 19.64 | B |
| | ATOM | 2942 | HG | SER | 260 | 18.255 | 51.324 | 28.441 | 1.00 | 0.00 | B |
| | ATOM | 2943 | C | SER | 260 | 15.619 | 49.794 | 29.109 | 1.00 | 16.77 | B |
| 20 | ATOM | 2944 | O | SER | 260 | 16.330 | 49.027 | 28.486 | 1.00 | 16.79 | B |
| | ATOM | 2945 | N | HIS | 261 | 14.292 | 49.719 | 29.083 | 1.00 | 20.77 | B |
| | ATOM | 2946 | H | HIS | 261 | 13.775 | 50.351 | 29.622 | 1.00 | 0.00 | B |
| | ATOM | 2947 | CA | HIS | 261 | 13.581 | 48.730 | 28.280 | 1.00 | 26.28 | B |
| | ATOM | 2948 | CB | HIS | 261 | 12.074 | 48.819 | 28.545 | 1.00 | 36.28 | B |
| 25 | ATOM | 2949 | CG | HIS | 261 | 11.565 | 47.849 | 29.564 | 1.00 | 47.66 | B |
| | ATOM | 2950 | CD2 | HIS | 261 | 10.832 | 46.717 | 29.426 | 1.00 | 49.49 | B |
| | ATOM | 2951 | ND1 | HIS | 261 | 11.764 | 48.015 | 30.919 | 1.00 | 51.66 | B |
| | ATOM | 2952 | HD1 | HIS | 261 | 12.252 | 48.757 | 31.331 | 1.00 | 0.00 | B |
| | ATOM | 2953 | CE1 | HIS | 261 | 11.170 | 47.034 | 31.575 | 1.00 | 50.93 | B |
| 30 | ATOM | 2954 | NE2 | HIS | 261 | 10.599 | 46.231 | 30.693 | 1.00 | 52.42 | B |
| | ATOM | 2955 | HE2 | HIS | 261 | 10.085 | 45.430 | 30.904 | 1.00 | 0.00 | B |
| | ATOM | 2956 | C | HIS | 261 | 13.836 | 49.169 | 26.854 | 1.00 | 23.53 | B |
| | ATOM | 2957 | O | HIS | 261 | 13.634 | 48.437 | 25.895 | 1.00 | 23.83 | B |
| | ATOM | 2958 | N | TYR | 262 | 14.292 | 50.405 | 26.767 | 1.00 | 22.41 | B |
| 35 | ATOM | 2959 | H | TYR | 262 | 14.447 | 50.886 | 27.607 | 1.00 | 0.00 | B |
| | ATOM | 2960 | CA | TYR | 262 | 14.581 | 51.112 | 25.537 | 1.00 | 22.32 | B |
| | ATOM | 2961 | CB | TYR | 262 | 14.348 | 52.594 | 25.795 | 1.00 | 29.85 | B |
| | ATOM | 2962 | CG | TYR | 262 | 13.305 | 53.169 | 24.914 | 1.00 | 35.37 | B |
| | ATOM | 2963 | CD1 | TYR | 262 | 12.587 | 54.264 | 25.316 | 1.00 | 29.84 | B |
| 40 | ATOM | 2964 | CE1 | TYR | 262 | 11.582 | 54.781 | 24.522 | 1.00 | 46.06 | B |
| | ATOM | 2965 | CD2 | TYR | 262 | 13.009 | 52.594 | 23.671 | 1.00 | 41.64 | B |
| | ATOM | 2966 | CE2 | TYR | 262 | 11.987 | 53.118 | 22.858 | 1.00 | 46.38 | B |
| | ATOM | 2967 | CZ | TYR | 262 | 11.281 | 54.224 | 23.302 | 1.00 | 41.00 | B |
| | ATOM | 2968 | OH | TYR | 262 | 10.252 | 54.782 | 22.570 | 1.00 | 44.86 | B |
| 45 | ATOM | 2969 | HH | TYR | 262 | 10.120 | 54.276 | 21.766 | 1.00 | 0.00 | B |
| | ATOM | 2970 | C | TYR | 262 | 15.981 | 50.955 | 24.943 | 1.00 | 21.72 | B |
| | ATOM | 2971 | O | TYR | 262 | 16.269 | 51.550 | 23.903 | 1.00 | 17.28 | B |
| | ATOM | 2972 | N | ASN | 263 | 16.839 | 50.201 | 25.628 | 1.00 | 23.04 | B |
| | ATOM | 2973 | H | ASN | 263 | 16.526 | 49.784 | 26.457 | 1.00 | 0.00 | B |
| 50 | ATOM | 2974 | CA | ASN | 263 | 18.222 | 49.950 | 25.220 | 1.00 | 24.13 | B |
| | ATOM | 2975 | CB | ASN | 263 | 18.634 | 48.513 | 25.584 | 1.00 | 29.95 | B |
| | ATOM | 2976 | CG | ASN | 263 | 18.971 | 48.335 | 27.058 | 1.00 | 36.99 | B |
| | ATOM | 2977 | OD1 | ASN | 263 | 18.731 | 49.210 | 27.886 | 1.00 | 41.66 | B |
| | ATOM | 2978 | ND2 | ASN | 263 | 19.528 | 47.181 | 27.384 | 1.00 | 40.94 | B |
| 55 | ATOM | 2979 | HD21 | ASN | 263 | 19.702 | 46.507 | 26.693 | 1.00 | 0.00 | B |
| | ATOM | 2980 | HD22 | ASN | 263 | 19.752 | 47.038 | 28.326 | 1.00 | 0.00 | B |
| | ATOM | 2981 | C | ASN | 263 | 18.543 | 50.136 | 23.736 | 1.00 | 23.55 | B |
| | ATOM | 2982 | O | ASN | 263 | 19.316 | 51.006 | 23.369 | 1.00 | 18.90 | B |
| | ATOM | 2983 | N | HIS | 264 | 17.958 | 49.279 | 22.900 | 1.00 | 23.91 | B |
| 60 | ATOM | 2984 | H | HIS | 264 | 17.341 | 48.618 | 23.274 | 1.00 | 0.00 | B |
| | ATOM | 2985 | CA | HIS | 264 | 18.189 | 49.276 | 21.458 | 1.00 | 26.11 | B |
| | ATOM | 2986 | CB | HIS | 264 | 17.205 | 48.308 | 20.778 | 1.00 | 23.47 | B |
| | ATOM | 2987 | CG | HIS | 264 | 15.766 | 48.685 | 20.947 | 1.00 | 22.25 | B |
| | ATOM | 2988 | CD2 | HIS | 264 | 14.846 | 48.294 | 21.863 | 1.00 | 24.90 | B |
| 65 | ATOM | 2989 | ND1 | HIS | 264 | 15.129 | 49.594 | 20.131 | 1.00 | 23.90 | B |
| | ATOM | 2990 | HD1 | HIS | 264 | 15.530 | 50.056 | 19.366 | 1.00 | 0.00 | B |
| | ATOM | 2991 | CE1 | HIS | 264 | 13.881 | 49.748 | 20.532 | 1.00 | 31.00 | B |
| | ATOM | 2992 | NE2 | HIS | 264 | 13.683 | 48.970 | 21.586 | 1.00 | 28.44 | B |
| | ATOM | 2993 | HE2 | HIS | 264 | 12.847 | 48.889 | 22.081 | 1.00 | 0.00 | B |
| 70 | ATOM | 2994 | C | HIS | 264 | 18.163 | 50.601 | 20.706 | 1.00 | 29.92 | B |
| | ATOM | 2995 | O | HIS | 264 | 18.712 | 50.710 | 19.614 | 1.00 | 31.12 | B |
| | ATOM | 2996 | N | ARG | 265 | 17.527 | 51.613 | 21.282 | 1.00 | 30.38 | B |
| | ATOM | 2997 | H | ARG | 265 | 17.125 | 51.493 | 22.161 | 1.00 | 0.00 | B |
| | ATOM | 2998 | CA | ARG | 265 | 17.435 | 52.905 | 20.619 | 1.00 | 33.48 | B |
| 70 | ATOM | 2999 | CB | ARG | 265 | 16.140 | 53.580 | 21.011 | 1.00 | 35.96 | B |
| | ATOM | 3000 | CG | ARG | 265 | 14.909 | 52.909 | 20.585 | 1.00 | 43.13 | B |
| | ATOM | 3001 | CD | ARG | 265 | 14.090 | 53.926 | 19.852 | 1.00 | 45.62 | B |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 3002 | NE | ARG | 265 | 13.403 | 54.838 | 20.755 | 1.00 | 41.09 | B |
| | ATOM | 3003 | HE | ARG | 265 | 13.054 | 54.478 | 21.594 | 1.00 | 0.00 | B |
| | ATOM | 3004 | CZ | ARG | 265 | 13.218 | 56.130 | 20.506 | 1.00 | 42.46 | B |
| | ATOM | 3005 | NH1 | ARG | 265 | 13.671 | 56.670 | 19.380 | 1.00 | 43.62 | B |
| | ATOM | 3006 | HH11 | ARG | 265 | 14.151 | 56.104 | 18.710 | 1.00 | 0.00 | B |
| | ATOM | 3007 | HH12 | ARG | 265 | 13.529 | 57.644 | 19.202 | 1.00 | 0.00 | B |
| | ATOM | 3008 | NH2 | ARG | 265 | 12.565 | 56.879 | 21.374 | 1.00 | 43.11 | B |
| 10 | ATOM | 3009 | HH21 | ARG | 265 | 12.206 | 56.472 | 22.213 | 1.00 | 0.00 | B |
| | ATOM | 3010 | HH22 | ARG | 265 | 12.426 | 57.852 | 21.189 | 1.00 | 0.00 | B |
| | ATOM | 3011 | C | ARG | 265 | 18.535 | 53.875 | 21.040 | 1.00 | 31.98 | B |
| | ATOM | 3012 | O | ARG | 265 | 18.666 | 54.954 | 20.443 | 1.00 | 25.36 | B |
| | ATOM | 3013 | N | LEU | 266 | 19.302 | 53.472 | 22.059 | 1.00 | 27.18 | B |
| | ATOM | 3014 | H | LEU | 266 | 19.231 | 52.547 | 22.360 | 1.00 | 0.00 | B |
| | ATOM | 3015 | CA | LEU | 266 | 20.303 | 54.346 | 22.685 | 1.00 | 26.54 | B |
| 15 | ATOM | 3016 | CB | LEU | 266 | 20.987 | 53.646 | 23.864 | 1.00 | 21.25 | B |
| | ATOM | 3017 | CG | LEU | 266 | 20.178 | 53.787 | 25.158 | 1.00 | 23.40 | B |
| | ATOM | 3018 | CD1 | LEU | 266 | 20.950 | 53.117 | 26.265 | 1.00 | 16.18 | B |
| | ATOM | 3019 | CD2 | LEU | 266 | 19.900 | 55.260 | 25.505 | 1.00 | 27.07 | B |
| | ATOM | 3020 | C | LEU | 266 | 21.337 | 54.990 | 21.809 | 1.00 | 28.09 | B |
| | ATOM | 3021 | O | LEU | 266 | 21.467 | 56.208 | 21.838 | 1.00 | 30.85 | B |
| | ATOM | 3022 | N | GLN | 267 | 22.045 | 54.199 | 21.031 | 1.00 | 29.76 | B |
| 20 | ATOM | 3023 | H | GLN | 267 | 21.873 | 53.236 | 21.016 | 1.00 | 0.00 | B |
| | ATOM | 3024 | CA | GLN | 267 | 23.086 | 54.733 | 20.162 | 1.00 | 29.56 | B |
| | ATOM | 3025 | CB | GLN | 267 | 23.692 | 53.605 | 19.344 | 1.00 | 36.52 | B |
| | ATOM | 3026 | CG | GLN | 267 | 23.964 | 52.362 | 20.169 | 1.00 | 50.23 | B |
| | ATOM | 3027 | CD | GLN | 267 | 23.778 | 51.084 | 19.380 | 1.00 | 58.15 | B |
| | ATOM | 3028 | OE1 | GLN | 267 | 23.350 | 50.056 | 19.919 | 1.00 | 60.56 | B |
| | ATOM | 3029 | NE2 | GLN | 267 | 24.100 | 51.138 | 18.089 | 1.00 | 62.36 | B |
| 25 | ATOM | 3030 | HE21 | GLN | 267 | 24.434 | 51.976 | 17.706 | 1.00 | 0.00 | B |
| | ATOM | 3031 | HE22 | GLN | 267 | 23.988 | 50.324 | 17.561 | 1.00 | 0.00 | B |
| | ATOM | 3032 | C | GLN | 267 | 22.556 | 55.825 | 19.245 | 1.00 | 31.18 | B |
| | ATOM | 3033 | O | GLN | 267 | 23.145 | 56.905 | 19.130 | 1.00 | 27.34 | B |
| | ATOM | 3034 | N | LYS | 268 | 21.443 | 55.540 | 18.582 | 1.00 | 29.62 | B |
| | ATOM | 3035 | H | LYS | 268 | 21.009 | 54.672 | 18.704 | 1.00 | 0.00 | B |
| | ATOM | 3036 | CA | LYS | 268 | 20.872 | 56.514 | 17.687 | 1.00 | 26.36 | B |
| 30 | ATOM | 3037 | CB | LYS | 268 | 19.650 | 55.937 | 16.976 | 1.00 | 29.19 | B |
| | ATOM | 3038 | CG | LYS | 268 | 19.037 | 56.897 | 15.952 | 1.00 | 37.26 | B |
| | ATOM | 3039 | CD | LYS | 268 | 20.002 | 57.194 | 14.800 | 1.00 | 37.93 | B |
| | ATOM | 3040 | CE | LYS | 268 | 19.555 | 56.514 | 13.516 | 1.00 | 45.23 | B |
| | ATOM | 3041 | NZ | LYS | 268 | 20.397 | 56.862 | 12.327 | 1.00 | 50.96 | B |
| | ATOM | 3042 | HZ1 | LYS | 268 | 21.379 | 56.574 | 12.501 | 1.00 | 0.00 | B |
| | ATOM | 3043 | HZ2 | LYS | 268 | 20.358 | 57.888 | 12.163 | | | |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 3075 | O | GLN | 271 | 24.067 | 62.496 | 17.509 | 1.00 | 16.78 | B |
| | ATOM | 3076 | N | ASP | 272 | 22.082 | 61.557 | 18.025 | 1.00 | 21.10 | B |
| | ATOM | 3077 | H | ASP | 272 | 21.615 | 60.756 | 18.343 | 1.00 | 0.00 | B |
| | ATOM | 3078 | CA | ASP | 272 | 21.325 | 62.718 | 17.650 | 1.00 | 17.66 | B |
| | ATOM | 3079 | CB | ASP | 272 | 19.848 | 62.340 | 17.563 | 1.00 | 21.71 | B |
| 10 | ATOM | 3080 | CG | ASP | 272 | 19.567 | 61.417 | 16.376 | 1.00 | 24.50 | B |
| | ATOM | 3081 | OD1 | ASP | 272 | 20.276 | 61.541 | 15.361 | 1.00 | 31.04 | B |
| | ATOM | 3082 | OD2 | ASP | 272 | 18.656 | 60.571 | 16.449 | 1.00 | 28.77 | B |
| | ATOM | 3083 | C | ASP | 272 | 21.593 | 63.832 | 18.656 | 1.00 | 17.80 | B |
| | ATOM | 3084 | O | ASP | 272 | 21.699 | 64.997 | 18.284 | 1.00 | 18.02 | B |
| 15 | ATOM | 3085 | N | CYS | 273 | 21.729 | 63.477 | 19.931 | 1.00 | 18.60 | B |
| | ATOM | 3086 | H | CYS | 273 | 21.636 | 62.537 | 20.187 | 1.00 | 0.00 | B |
| | ATOM | 3087 | CA | CYS | 273 | 22.022 | 64.488 | 20.945 | 1.00 | 20.63 | B |
| | ATOM | 3088 | CB | CYS | 273 | 22.050 | 63.867 | 22.347 | 1.00 | 16.54 | B |
| | ATOM | 3089 | SG | CYS | 273 | 20.445 | 63.515 | 23.095 | 1.00 | 35.11 | B |
| 20 | ATOM | 3090 | C | CYS | 273 | 23.396 | 65.085 | 20.641 | 1.00 | 23.93 | B |
| | ATOM | 3091 | O | CYS | 273 | 23.579 | 66.305 | 20.707 | 1.00 | 21.34 | B |
| | ATOM | 3092 | N | GLU | 274 | 24.346 | 64.212 | 20.304 | 1.00 | 21.52 | B |
| | ATOM | 3093 | H | GLU | 274 | 24.114 | 63.261 | 20.261 | 1.00 | 0.00 | B |
| | ATOM | 3094 | CA | GLU | 274 | 25.723 | 64.601 | 19.993 | 1.00 | 25.93 | B |
| 25 | ATOM | 3095 | CB | GLU | 274 | 26.523 | 63.355 | 19.575 | 1.00 | 25.37 | B |
| | ATOM | 3096 | CG | GLU | 274 | 28.017 | 63.412 | 19.847 | 1.00 | 33.76 | B |
| | ATOM | 3097 | CD | GLU | 274 | 28.381 | 64.114 | 21.149 | 1.00 | 35.86 | B |
| | ATOM | 3098 | OE1 | GLU | 274 | 29.384 | 64.855 | 21.154 | 1.00 | 39.26 | B |
| | ATOM | 3099 | OE2 | GLU | 274 | 27.682 | 63.929 | 22.164 | 1.00 | 31.65 | B |
| 30 | ATOM | 3100 | C | GLU | 274 | 25.801 | 65.667 | 18.896 | 1.00 | 27.29 | B |
| | ATOM | 3101 | O | GLU | 274 | 26.479 | 66.692 | 19.055 | 1.00 | 21.91 | B |
| | ATOM | 3102 | N | ASP | 275 | 25.110 | 65.409 | 17.786 | 1.00 | 25.89 | B |
| | ATOM | 3103 | H | ASP | 275 | 24.605 | 64.571 | 17.736 | 1.00 | 0.00 | B |
| | ATOM | 3104 | CA | ASP | 275 | 25.069 | 66.319 | 16.635 | 1.00 | 29.31 | B |
| 35 | ATOM | 3105 | CB | ASP | 275 | 24.320 | 65.655 | 15.471 | 1.00 | 28.05 | B |
| | ATOM | 3106 | CG | ASP | 275 | 25.031 | 64.420 | 14.938 | 1.00 | 37.38 | B |
| | ATOM | 3107 | OD1 | ASP | 275 | 26.257 | 64.293 | 15.145 | 1.00 | 41.51 | B |
| | ATOM | 3108 | OD2 | ASP | 275 | 24.360 | 63.575 | 14.305 | 1.00 | 34.32 | B |
| | ATOM | 3109 | C | ASP | 275 | 24.408 | 67.674 | 16.939 | 1.00 | 29.09 | B |
| 40 | ATOM | 3110 | O | ASP | 275 | 24.678 | 68.679 | 16.268 | 1.00 | 22.13 | B |
| | ATOM | 3111 | N | GLU | 276 | 23.529 | 67.688 | 17.935 | 1.00 | 30.74 | B |
| | ATOM | 3112 | H | GLU | 276 | 23.353 | 66.859 | 18.423 | 1.00 | 0.00 | B |
| | ATOM | 3113 | CA | GLU | 276 | 22.817 | 68.901 | 18.327 | 1.00 | 32.15 | B |
| | ATOM | 3114 | CB | GLU | 276 | 21.403 | 68.554 | 18.792 | 1.00 | 31.31 | B |
| 45 | ATOM | 3115 | CG | GLU | 276 | 20.404 | 68.622 | 17.654 | 1.00 | 35.70 | B |
| | ATOM | 3116 | CD | GLU | 276 | 19.015 | 68.175 | 18.049 | 1.00 | 42.31 | B |
| | ATOM | 3117 | OE1 | GLU | 276 | 18.415 | 67.389 | 17.284 | 1.00 | 40.50 | B |
| | ATOM | 3118 | OE2 | GLU | 276 | 18.521 | 68.606 | 19.115 | 1.00 | 46.76 | B |
| | ATOM | 3119 | C | GLU | 276 | 23.606 | 69.557 | 19.431 | 1.00 | 29.44 | B |
| 50 | ATOM | 3120 | O | GLU | 276 | 23.234 | 70.604 | 19.968 | 1.00 | 24.35 | B |
| | ATOM | 3121 | N | ASN | 277 | 24.727 | 68.918 | 19.744 | 1.00 | 28.11 | B |
| | ATOM | 3122 | H | ASN | 277 | 24.942 | 68.087 | 19.272 | 1.00 | 0.00 | B |
| | ATOM | 3123 | CA | ASN | 277 | 25.644 | 69.401 | 20.757 | 1.00 | 29.61 | B |
| | ATOM | 3124 | CB | ASN | 277 | 26.309 | 70.682 | 20.271 | 1.00 | 32.09 | B |
| 55 | ATOM | 3125 | CG | ASN | 277 | 27.387 | 70.398 | 19.252 | 1.00 | 38.92 | B |
| | ATOM | 3126 | OD1 | ASN | 277 | 28.455 | 69.880 | 19.597 | 1.00 | 38.13 | B |
| | ATOM | 3127 | ND2 | ASN | 277 | 27.113 | 70.712 | 17.989 | 1.00 | 39.28 | B |
| | ATOM | 3128 | HD21 | ASN | 277 | 26.245 | 71.104 | 17.760 | 1.00 | 0.00 | B |
| | ATOM | 3129 | HD22 | ASN | 277 | 27.804 | 70.534 | 17.319 | 1.00 | 0.00 | B |
| 60 | ATOM | 3130 | C | ASN | 277 | 25.023 | 69.617 | 22.111 | 1.00 | 27.06 | B |
| | ATOM | 3131 | O | ASN | 277 | 25.118 | 70.691 | 22.693 | 1.00 | 28.18 | B |
| | ATOM | 3132 | N | ILE | 278 | 24.390 | 68.572 | 22.613 | 1.00 | 22.45 | B |
| | ATOM | 3133 | H | ILE | 278 | 24.339 | 67.740 | 22.096 | 1.00 | 0.00 | B |
| | ATOM | 3134 | CA | ILE | 278 | 23.775 | 68.640 | 23.909 | 1.00 | 18.31 | B |
| 65 | ATOM | 3135 | CB | ILE | 278 | 22.422 | 67.904 | 23.899 | 1.00 | 14.49 | B |
| | ATOM | 3136 | CG2 | ILE | 278 | 21.895 | 67.787 | 25.306 | 1.00 | 12.68 | B |
| | ATOM | 3137 | CG1 | ILE | 278 | 21.454 | 68.639 | 22.962 | 1.00 | 17.11 | B |
| | ATOM | 3138 | CD1 | ILE | 278 | 20.093 | 68.024 | 22.870 | 1.00 | 16.07 | B |
| | ATOM | 3139 | C | ILE | 278 | 24.728 | 67.978 | 24.903 | 1.00 | 18.85 | B |
| 70 | ATOM | 3140 | O | ILE | 278 | 25.052 | 66.802 | 24.767 | 1.00 | 17.29 | B |
| | ATOM | 3141 | N | GLN | 279 | 25.180 | 68.738 | 25.896 | 1.00 | 15.07 | B |
| | ATOM | 3142 | H | GLN | 279 | 24.907 | 69.676 | 25.956 | 1.00 | 0.00 | B |
| | ATOM | 3143 | CA | GLN | 279 | 26.071 | 68.182 | 26.891 | 1.00 | 20.54 | B |
| | ATOM | 3144 | CB | GLN | 279 | 26.788 | 69.299 | 27.636 | 1.00 | 22.04 | B |
| | ATOM | 3145 | CG | GLN | 279 | 28.008 | 68.836 | 28.428 | 1.00 | 25.39 | B |
| | ATOM | 3146 | CD | GLN | 279 | 28.683 | 69.984 | 29.146 | 1.00 | 25.91 | B |
| | ATOM | 3147 | OE1 | GLN | 279 | 29.500 | 69.777 | 30.040 | 1.00 | 26.55 | B |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 3148 | NE2 | GLN | 279 | 28.340 | 71.208 | 28.758 | 1.00 | 23.93 | B |
| | ATOM | 3149 | HE21 | GLN | 279 | 27.685 | 71.328 | 28.040 | 1.00 | 0.00 | B |
| | ATOM | 3150 | HE22 | GLN | 279 | 28.769 | 71.963 | 29.211 | 1.00 | 0.00 | B |
| | ATOM | 3151 | C | GLN | 279 | 25.253 | 67.347 | 27.866 | 1.00 | 17.77 | B |
| | ATOM | 3152 | O | GLN | 279 | 24.310 | 67.847 | 28.475 | 1.00 | 21.13 | B |
| 10 | ATOM | 3153 | N | ARG | 280 | 25.620 | 66.081 | 28.025 | 1.00 | 19.35 | B |
| | ATOM | 3154 | H | ARG | 280 | 26.398 | 65.742 | 27.538 | 1.00 | 0.00 | B |
| | ATOM | 3155 | CA | ARG | 280 | 24.880 | 65.184 | 28.913 | 1.00 | 17.76 | B |
| | ATOM | 3156 | CB | ARG | 280 | 24.285 | 64.007 | 28.123 | 1.00 | 13.32 | B |
| | ATOM | 3157 | CG | ARG | 280 | 24.065 | 64.255 | 26.641 | 1.00 | 16.90 | B |
| 15 | ATOM | 3158 | CD | ARG | 280 | 23.912 | 62.956 | 25.872 | 1.00 | 12.99 | B |
| | ATOM | 3159 | NE | ARG | 280 | 25.175 | 62.404 | 25.368 | 1.00 | 14.94 | B |
| | ATOM | 3160 | HE | ARG | 280 | 25.533 | 61.605 | 25.802 | 1.00 | 0.00 | B |
| | ATOM | 3161 | CZ | ARG | 280 | 25.866 | 62.931 | 24.363 | 1.00 | 18.57 | B |
| | ATOM | 3162 | NH1 | ARG | 280 | 25.421 | 64.025 | 23.754 | 1.00 | 16.91 | B |
| 20 | ATOM | 3163 | HH11 | ARG | 280 | 24.569 | 64.453 | 24.058 | 1.00 | 0.00 | B |
| | ATOM | 3164 | HH12 | ARG | 280 | 25.937 | 64.421 | 22.996 | 1.00 | 0.00 | B |
| | ATOM | 3165 | NH2 | ARG | 280 | 27.005 | 62.370 | 23.965 | 1.00 | 12.64 | B |
| | ATOM | 3166 | HH21 | ARG | 280 | 27.344 | 61.552 | 24.430 | 1.00 | 0.00 | B |
| | ATOM | 3167 | HH22 | ARG | 280 | 27.521 | 62.763 | 23.211 | 1.00 | 0.00 | B |
| 25 | ATOM | 3168 | C | ARG | 280 | 25.628 | 64.601 | 30.111 | 1.00 | 16.54 | B |
| | ATOM | 3169 | O | ARG | 280 | 26.644 | 63.912 | 29.968 | 1.00 | 18.85 | B |
| | ATOM | 3170 | N | PHE | 281 | 25.099 | 64.893 | 31.288 | 1.00 | 14.11 | B |
| | ATOM | 3171 | H | PHE | 281 | 24.324 | 65.492 | 31.315 | 1.00 | 0.00 | B |
| | ATOM | 3172 | CA | PHE | 281 | 25.611 | 64.374 | 32.543 | 1.00 | 13.98 | B |
| 30 | ATOM | 3173 | CB | PHE | 281 | 25.610 | 65.452 | 33.632 | 1.00 | 20.05 | B |
| | ATOM | 3174 | CG | PHE | 281 | 26.572 | 66.572 | 33.394 | 1.00 | 23.08 | B |
| | ATOM | 3175 | CD1 | PHE | 281 | 26.213 | 67.660 | 32.606 | 1.00 | 22.44 | B |
| | ATOM | 3176 | CD2 | PHE | 281 | 27.822 | 66.564 | 33.998 | 1.00 | 20.52 | B |
| | ATOM | 3177 | CE1 | PHE | 281 | 27.086 | 68.732 | 32.426 | 1.00 | 23.69 | B |
| 35 | ATOM | 3178 | CE2 | PHE | 281 | 28.702 | 67.628 | 33.826 | 1.00 | 19.90 | B |
| | ATOM | 3179 | CZ | PHE | 281 | 28.328 | 68.718 | 33.038 | 1.00 | 22.07 | B |
| | ATOM | 3180 | C | PHE | 281 | 24.570 | 63.306 | 32.929 | 1.00 | 16.85 | B |
| | ATOM | 3181 | O | PHE | 281 | 23.370 | 63.589 | 32.962 | 1.00 | 17.22 | B |
| | ATOM | 3182 | N | SER | 282 | 25.022 | 62.095 | 33.231 | 1.00 | 14.65 | B |
| 40 | ATOM | 3183 | H | SER | 282 | 25.984 | 61.920 | 33.203 | 1.00 | 0.00 | B |
| | ATOM | 3184 | CA | SER | 282 | 24.104 | 61.030 | 33.605 | 1.00 | 14.06 | B |
| | ATOM | 3185 | CB | SER | 282 | 24.152 | 59.884 | 32.578 | 1.00 | 11.06 | B |
| | ATOM | 3186 | OG | SER | 282 | 25.449 | 59.298 | 32.482 | 1.00 | 18.85 | B |
| | ATOM | 3187 | HG | SER | 282 | 25.433 | 58.594 | 31.836 | 1.00 | 0.00 | B |
| 45 | ATOM | 3188 | C | SER | 282 | 24.449 | 60.516 | 34.984 | 1.00 | 15.44 | B |
| | ATOM | 3189 | O | SER | 282 | 25.631 | 60.359 | 35.310 | 1.00 | 22.28 | B |
| | ATOM | 3190 | N | ILE | 283 | 23.413 | 60.278 | 35.787 | 1.00 | 16.47 | B |
| | ATOM | 3191 | H | ILE | 283 | 22.513 | 60.444 | 35.442 | 1.00 | 0.00 | B |
| | ATOM | 3192 | CA | ILE | 283 | 23.541 | 59.776 | 37.152 | 1.00 | 12.03 | B |
| 50 | ATOM | 3193 | CB | ILE | 283 | 22.870 | 60.730 | 38.164 | 1.00 | 13.63 | B |
| | ATOM | 3194 | CG2 | ILE | 283 | 22.863 | 60.095 | 39.532 | 1.00 | 11.53 | B |
| | ATOM | 3195 | CG1 | ILE | 283 | 23.606 | 62.072 | 38.237 | 1.00 | 18.66 | B |
| | ATOM | 3196 | CD1 | ILE | 283 | 23.280 | 63.039 | 37.120 | 1.00 | 14.72 | B |
| | ATOM | 3197 | C | ILE | 283 | 22.842 | 58.403 | 37.283 | 1.00 | 20.66 | B |
| 55 | ATOM | 3198 | O | ILE | 283 | 21.623 | 58.291 | 37.068 | 1.00 | 19.36 | B |
| | ATOM | 3199 | N | ALA | 284 | 23.617 | 57.369 | 37.616 | 1.00 | 18.27 | B |
| | ATOM | 3200 | H | ALA | 284 | 24.579 | 57.514 | 37.731 | 1.00 | 0.00 | B |
| | ATOM | 3201 | CA | ALA | 284 | 23.082 | 56.022 | 37.814 | 1.00 | 16.02 | B |
| | ATOM | 3202 | CB | ALA | 284 | 24.000 | 54.974 | 37.196 | 1.00 | 17.51 | B |
| 60 | ATOM | 3203 | C | ALA | 284 | 22.963 | 55.767 | 39.299 | 1.00 | 18.28 | B |
| | ATOM | 3204 | O | ALA | 284 | 23.956 | 55.892 | 40.018 | 1.00 | 22.88 | B |
| | ATOM | 3205 | N | ILE | 285 | 21.753 | 55.430 | 39.764 | 1.00 | 19.46 | B |
| | ATOM | 3206 | H | ILE | 285 | 21.001 | 55.378 | 39.139 | 1.00 | 0.00 | B |
| | ATOM | 3207 | CA | ILE | 285 | 21.523 | 55.137 | 41.182 | 1.00 | 20.18 | B |
| 65 | ATOM | 3208 | CB | ILE | 285 | 20.188 | 55.716 | 41.703 | 1.00 | 19.17 | B |
| | ATOM | 3209 | CG2 | ILE | 285 | 19.893 | 55.174 | 43.103 | 1.00 | 17.01 | B |
| | ATOM | 3210 | CG1 | ILE | 285 | 20.256 | 57.235 | 41.762 | 1.00 | 17.37 | B |
| | ATOM | 3211 | CD1 | ILE | 285 | 19.131 | 57.923 | 41.023 | 1.00 | 18.02 | B |
| | ATOM | 3212 | C | ILE | 285 | 21.469 | 53.621 | 41.280 | 1.00 | 20.23 | B |
| 70 | ATOM | 3213 | O | ILE | 285 | 20.615 | 52.986 | 40.659 | 1.00 | 20.26 | B |
| | ATOM | 3214 | N | LEU | 286 | 22.384 | 53.045 | 42.052 | 1.00 | 17.07 | B |
| | ATOM | 3215 | H | LEU | 286 | 23.012 | 53.610 | 42.549 | 1.00 | 0.00 | B |
| | ATOM | 3216 | CA | LEU | 286 | 22.471 | 51.602 | 42.176 | 1.00 | 19.43 | B |
| | ATOM | 3217 | CB | LEU | 286 | 23.949 | 51.171 | 42.263 | 1.00 | 19.07 | B |
| | ATOM | 3218 | CG | LEU | 286 | 25.035 | 51.649 | 41.276 | 1.00 | 17.49 | B |
| | ATOM | 3219 | CD1 | LEU | 286 | 25.830 | 50.442 | 40.797 | 1.00 | 12.99 | B |
| | ATOM | 3220 | CD2 | LEU | 286 | 24.431 | 52.420 | 40.099 | 1.00 | 10.34 | B |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 3221 | C | LEU | 286 | 21.722 | 51.058 | 43.382 | 1.00 | 21.59 | B |
| | ATOM | 3222 | O | LEU | 286 | 21.885 | 49.895 | 43.742 | 1.00 | 23.43 | B |
| | ATOM | 3223 | N | GLY | 287 | 20.899 | 51.903 | 43.997 | 1.00 | 21.97 | B |
| | ATOM | 3224 | H | GLY | 287 | 20.792 | 52.812 | 43.647 | 1.00 | 0.00 | B |
| | ATOM | 3225 | CA | GLY | 287 | 20.158 | 51.493 | 45.173 | 1.00 | 19.38 | B |
| 10 | ATOM | 3226 | C | GLY | 287 | 19.312 | 50.236 | 45.051 | 1.00 | 23.15 | B |
| | ATOM | 3227 | O | GLY | 287 | 19.575 | 49.221 | 45.708 | 1.00 | 20.35 | B |
| | ATOM | 3228 | N | HIS | 288 | 18.285 | 50.308 | 44.215 | 1.00 | 17.51 | B |
| | ATOM | 3229 | H | HIS | 288 | 18.130 | 51.137 | 43.713 | 1.00 | 0.00 | B |
| | ATOM | 3230 | CA | HIS | 288 | 17.387 | 49.196 | 44.027 | 1.00 | 14.47 | B |
| 15 | ATOM | 3231 | CB | HIS | 288 | 16.298 | 49.571 | 43.042 | 1.00 | 14.52 | B |
| | ATOM | 3232 | CG | HIS | 288 | 15.289 | 48.495 | 42.825 | 1.00 | 15.66 | B |
| | ATOM | 3233 | CD2 | HIS | 288 | 15.157 | 47.585 | 41.826 | 1.00 | 6.58 | B |
| | ATOM | 3234 | ND1 | HIS | 288 | 14.289 | 48.220 | 43.731 | 1.00 | 10.26 | B |
| | ATOM | 3235 | HD1 | HIS | 288 | 14.116 | 48.715 | 44.551 | 1.00 | 0.00 | B |
| 20 | ATOM | 3236 | CE1 | HIS | 288 | 13.575 | 47.198 | 43.293 | 1.00 | 16.43 | B |
| | ATOM | 3237 | NE2 | HIS | 288 | 14.083 | 46.794 | 42.141 | 1.00 | 11.36 | B |
| | ATOM | 3238 | HE2 | HIS | 288 | 13.751 | 46.056 | 41.599 | 1.00 | 0.00 | B |
| | ATOM | 3239 | C | HIS | 288 | 18.086 | 47.939 | 43.532 | 1.00 | 20.49 | B |
| | ATOM | 3240 | O | HIS | 288 | 17.786 | 46.833 | 43.982 | 1.00 | 21.10 | B |
| 25 | ATOM | 3241 | N | TYR | 289 | 19.007 | 48.117 | 42.595 | 1.00 | 20.56 | B |
| | ATOM | 3242 | H | TYR | 289 | 19.202 | 49.023 | 42.276 | 1.00 | 0.00 | B |
| | ATOM | 3243 | CA | TYR | 289 | 19.733 | 46.995 | 42.034 | 1.00 | 18.95 | B |
| | ATOM | 3244 | CB | TYR | 289 | 20.740 | 47.489 | 41.004 | 1.00 | 16.43 | B |
| | ATOM | 3245 | CG | TYR | 289 | 20.221 | 47.446 | 39.597 | 1.00 | 16.33 | B |
| 30 | ATOM | 3246 | CD1 | TYR | 289 | 19.048 | 48.104 | 39.264 | 1.00 | 14.79 | B |
| | ATOM | 3247 | CE1 | TYR | 289 | 18.563 | 48.086 | 37.978 | 1.00 | 23.36 | B |
| | ATOM | 3248 | CD2 | TYR | 289 | 20.907 | 46.757 | 38.592 | 1.00 | 18.79 | B |
| | ATOM | 3249 | CE2 | TYR | 289 | 20.428 | 46.733 | 37.287 | 1.00 | 18.41 | B |
| | ATOM | 3250 | CZ | TYR | 289 | 19.252 | 47.409 | 36.991 | 1.00 | 22.68 | B |
| 35 | ATOM | 3251 | OH | TYR | 289 | 18.755 | 47.437 | 35.716 | 1.00 | 18.85 | B |
| | ATOM | 3252 | HH | TYR | 289 | 17.943 | 47.954 | 35.703 | 1.00 | 0.00 | B |
| | ATOM | 3253 | C | TYR | 289 | 20.467 | 46.221 | 43.120 | 1.00 | 16.62 | B |
| | ATOM | 3254 | O | TYR | 289 | 20.383 | 44.995 | 43.190 | 1.00 | 16.84 | B |
| | ATOM | 3255 | N | ASN | 290 | 21.182 | 46.940 | 43.976 | 1.00 | 14.38 | B |
| 40 | ATOM | 3256 | H | ASN | 290 | 21.203 | 47.921 | 43.912 | 1.00 | 0.00 | B |
| | ATOM | 3257 | CA | ASN | 290 | 21.927 | 46.254 | 45.007 | 1.00 | 16.73 | B |
| | ATOM | 3258 | CB | ASN | 290 | 23.029 | 47.167 | 45.546 | 1.00 | 16.82 | B |
| | ATOM | 3259 | CG | ASN | 290 | 24.202 | 47.282 | 44.575 | 1.00 | 23.04 | B |
| | ATOM | 3260 | OD1 | ASN | 290 | 24.477 | 46.361 | 43.788 | 1.00 | 17.55 | B |
| 45 | ATOM | 3261 | ND2 | ASN | 290 | 24.892 | 48.410 | 44.618 | 1.00 | 21.77 | B |
| | ATOM | 3262 | HD21 | ASN | 290 | 24.637 | 49.116 | | | | |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 3294 | ND2 | ASN | 293 | 23.286 | 39.667 | 44.580 | 1.00 | 16.64 | B |
| | ATOM | 3295 | HD21 | ASN | 293 | 23.321 | 40.544 | 45.016 | 1.00 | 0.00 | B |
| | ATOM | 3296 | HD22 | ASN | 293 | 24.090 | 39.158 | 44.353 | 1.00 | 0.00 | B |
| | ATOM | 3297 | C | ASN | 293 | 20.851 | 41.290 | 42.578 | 1.00 | 24.68 | B |
| | ATOM | 3298 | O | ASN | 293 | 20.937 | 40.199 | 42.009 | 1.00 | 25.78 | B |
| 10 | ATOM | 3299 | N | LEU | 294 | 20.690 | 42.432 | 41.917 | 1.00 | 27.45 | B |
| | ATOM | 3300 | H | LEU | 294 | 20.582 | 43.268 | 42.415 | 1.00 | 0.00 | B |
| | ATOM | 3301 | CA | LEU | 294 | 20.666 | 42.454 | 40.457 | 1.00 | 26.46 | B |
| | ATOM | 3302 | CB | LEU | 294 | 19.696 | 43.514 | 39.920 | 1.00 | 21.98 | B |
| | ATOM | 3303 | CG | LEU | 294 | 18.249 | 43.549 | 40.402 | 1.00 | 33.38 | B |
| 15 | ATOM | 3304 | CD1 | LEU | 294 | 17.464 | 44.534 | 39.538 | 1.00 | 32.24 | B |
| | ATOM | 3305 | CD2 | LEU | 294 | 17.639 | 42.177 | 40.334 | 1.00 | 27.44 | B |
| | ATOM | 3306 | C | LEU | 294 | 22.063 | 42.822 | 39.984 | 1.00 | 24.21 | B |
| | ATOM | 3307 | O | LEU | 294 | 22.709 | 43.685 | 40.571 | 1.00 | 23.66 | B |
| | ATOM | 3308 | N | SER | 295 | 22.526 | 42.174 | 38.924 | 1.00 | 23.08 | B |
| 20 | ATOM | 3309 | H | SER | 295 | 21.984 | 41.469 | 38.512 | 1.00 | 0.00 | B |
| | ATOM | 3310 | CA | SER | 295 | 23.833 | 42.497 | 38.366 | 1.00 | 24.49 | B |
| | ATOM | 3311 | CB | SER | 295 | 24.211 | 41.481 | 37.284 | 1.00 | 22.71 | B |
| | ATOM | 3312 | OG | SER | 295 | 25.057 | 42.058 | 36.307 | 1.00 | 28.77 | B |
| | ATOM | 3313 | HG | SER | 295 | 25.856 | 42.370 | 36.726 | 1.00 | 0.00 | B |
| 25 | ATOM | 3314 | C | SER | 295 | 23.724 | 43.909 | 37.759 | 1.00 | 20.29 | B |
| | ATOM | 3315 | O | SER | 295 | 22.815 | 44.187 | 36.983 | 1.00 | 18.00 | B |
| | ATOM | 3316 | N | THR | 296 | 24.660 | 44.777 | 38.118 | 1.00 | 16.49 | B |
| | ATOM | 3317 | H | THR | 296 | 25.372 | 44.479 | 38.724 | 1.00 | 0.00 | B |
| | ATOM | 3318 | CA | THR | 296 | 24.679 | 46.166 | 37.653 | 1.00 | 18.66 | B |
| 30 | ATOM | 3319 | CB | THR | 296 | 25.023 | 47.101 | 38.804 | 1.00 | 19.68 | B |
| | ATOM | 3320 | OG1 | THR | 296 | 26.258 | 46.675 | 39.393 | 1.00 | 19.06 | B |
| | ATOM | 3321 | HG1 | THR | 296 | 26.162 | 45.778 | 39.722 | 1.00 | 0.00 | B |
| | ATOM | 3322 | CG2 | THR | 296 | 23.927 | 47.060 | 39.863 | 1.00 | 22.45 | B |
| | ATOM | 3323 | C | THR | 296 | 25.664 | 46.470 | 36.535 | 1.00 | 19.63 | B |
| 35 | ATOM | 3324 | O | THR | 296 | 25.808 | 47.626 | 36.136 | 1.00 | 17.70 | B |
| | ATOM | 3325 | N | GLU | 297 | 26.324 | 45.439 | 36.016 | 1.00 | 21.20 | B |
| | ATOM | 3326 | H | GLU | 297 | 26.131 | 44.536 | 36.341 | 1.00 | 0.00 | B |
| | ATOM | 3327 | CA | GLU | 297 | 27.325 | 45.622 | 34.972 | 1.00 | 21.26 | B |
| | ATOM | 3328 | CB | GLU | 297 | 28.042 | 44.291 | 34.710 | 1.00 | 30.39 | B |
| 40 | ATOM | 3329 | CG | GLU | 297 | 29.004 | 43.863 | 35.838 | 1.00 | 39.46 | B |
| | ATOM | 3330 | CD | GLU | 297 | 28.305 | 43.191 | 37.015 | 1.00 | 41.75 | B |
| | ATOM | 3331 | OE1 | GLU | 297 | 27.330 | 42.455 | 36.778 | 1.00 | 45.39 | B |
| | ATOM | 3332 | OE2 | GLU | 297 | 28.735 | 43.392 | 38.173 | 1.00 | 35.85 | B |
| | ATOM | 3333 | C | GLU | 297 | 26.789 | 46.210 | 33.675 | 1.00 | 22.11 | B |
| 45 | ATOM | 3334 | O | GLU | 297 | 27.344 | 47.184 | 33.151 | 1.00 | 18.94 | B |
| | ATOM | 3335 | N | LYS | 298 | 25.717 | 45.622 | 33.153 | 1.00 | 15.26 | B |
| | ATOM | 3336 | H | LYS | 298 | 25.330 | 44.845 | 33.608 | 1.00 | 0.00 | B |
| | ATOM | 3337 | CA | LYS | 298 | 25.105 | 46.107 | 31.925 | 1.00 | 17.69 | B |
| | ATOM | 3338 | CB | LYS | 298 | 23.958 | 45.163 | 31.500 | 1.00 | 22.54 | B |
| 50 | ATOM | 3339 | CG | LYS | 298 | 23.297 | 45.486 | 30.151 | 1.00 | 16.04 | B |
| | ATOM | 3340 | CD | LYS | 298 | 22.093 | 44.565 | 29.903 | 1.00 | 15.19 | B |
| | ATOM | 3341 | CE | LYS | 298 | 21.795 | 44.409 | 28.415 | 1.00 | 24.32 | B |
| | ATOM | 3342 | NZ | LYS | 298 | 20.353 | 44.064 | 28.147 | 1.00 | 31.08 | B |
| | ATOM | 3343 | HZ1 | LYS | 298 | 19.741 | 44.822 | 28.518 | 1.00 | 0.00 | B |
| 55 | ATOM | 3344 | HZ2 | LYS | 298 | 20.114 | 43.169 | 28.620 | 1.00 | 0.00 | B |
| | ATOM | 3345 | HZ3 | LYS | 298 | 20.202 | 43.968 | 27.124 | 1.00 | 0.00 | B |
| | ATOM | 3346 | C | LYS | 298 | 24.556 | 47.506 | 32.172 | 1.00 | 14.71 | B |
| | ATOM | 3347 | O | LYS | 298 | 24.718 | 48.410 | 31.356 | 1.00 | 19.72 | B |
| | ATOM | 3348 | N | PHE | 299 | 23.915 | 47.659 | 33.322 | 1.00 | 19.20 | B |
| 60 | ATOM | 3349 | H | PHE | 299 | 23.860 | 46.891 | 33.929 | 1.00 | 0.00 | B |
| | ATOM | 3350 | CA | PHE | 299 | 23.283 | 48.912 | 33.744 | 1.00 | 16.23 | B |
| | ATOM | 3351 | CB | PHE | 299 | 22.600 | 48.673 | 35.110 | 1.00 | 15.69 | B |
| | ATOM | 3352 | CG | PHE | 299 | 22.135 | 49.920 | 35.826 | 1.00 | 17.83 | B |
| | ATOM | 3353 | CD1 | PHE | 299 | 21.724 | 51.058 | 35.127 | 1.00 | 17.90 | B |
| 65 | ATOM | 3354 | CD2 | PHE | 299 | 22.110 | 49.949 | 37.216 | 1.00 | 17.55 | B |
| | ATOM | 3355 | CE1 | PHE | 299 | 21.303 | 52.191 | 35.802 | 1.00 | 15.38 | B |
| | ATOM | 3356 | CE2 | PHE | 299 | 21.687 | 51.087 | 37.897 | 1.00 | 26.58 | B |
| | ATOM | 3357 | CZ | PHE | 299 | 21.282 | 52.213 | 37.179 | 1.00 | 19.56 | B |
| | ATOM | 3358 | C | PHE | 299 | 24.276 | 50.079 | 33.818 | 1.00 | 17.61 | B |
| 70 | ATOM | 3359 | O | PHE | 299 | 24.087 | 51.099 | 33.163 | 1.00 | 16.95 | B |
| | ATOM | 3360 | N | VAL | 300 | 25.327 | 49.914 | 34.617 | 1.00 | 17.22 | B |
| | ATOM | 3361 | H | VAL | 300 | 25.433 | 49.066 | 35.094 | 1.00 | 0.00 | B |
| | ATOM | 3362 | CA | VAL | 300 | 26.322 | 50.959 | 34.801 | 1.00 | 18.55 | B |
| | ATOM | 3363 | CB | VAL | 300 | 27.421 | 50.492 | 35.773 | 1.00 | 16.60 | B |
| | ATOM | 3364 | CG1 | VAL | 300 | 28.724 | 51.220 | 35.492 | 1.00 | 21.52 | B |
| | ATOM | 3365 | CG2 | VAL | 300 | 26.974 | 50.723 | 37.195 | 1.00 | 19.24 | B |
| | ATOM | 3366 | C | VAL | 300 | 26.941 | 51.382 | 33.480 | 1.00 | 17.23 | B |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|---|
| | ATOM | 3367 | O | VAL | 300 | 27.075 | 52.569 | 33.198 | 1.00 | 15.55 | B |
| | ATOM | 3368 | N | GLU | 301 | 27.293 | 50.400 | 32.665 | 1.00 | 15.45 | B |
| | ATOM | 3369 | H | GLU | 301 | 27.145 | 49.471 | 32.939 | 1.00 | 0.00 | B |
| 5 | ATOM | 3370 | CA | GLU | 301 | 27.892 | 50.674 | 31.374 | 1.00 | 20.07 | B |
| | ATOM | 3371 | CB | GLU | 301 | 28.282 | 49.349 | 30.708 | 1.00 | 25.34 | B |
| | ATOM | 3372 | CG | GLU | 301 | 28.738 | 49.477 | 29.274 | 1.00 | 40.60 | B |
| | ATOM | 3373 | CD | GLU | 301 | 27.589 | 49.413 | 28.283 | 1.00 | 50.61 | B |
| | ATOM | 3374 | OE1 | GLU | 301 | 26.510 | 48.871 | 28.633 | 1.00 | 56.16 | B |
| | ATOM | 3375 | OE2 | GLU | 301 | 27.771 | 49.908 | 27.146 | 1.00 | 54.98 | B |
| 10 | ATOM | 3376 | C | GLU | 301 | 26.956 | 51.483 | 30.457 | 1.00 | 22.33 | B |
| | ATOM | 3377 | O | GLU | 301 | 27.413 | 52.316 | 29.663 | 1.00 | 18.68 | B |
| | ATOM | 3378 | N | GLU | 302 | 25.652 | 51.235 | 30.573 | 1.00 | 21.56 | B |
| | ATOM | 3379 | H | GLU | 302 | 25.349 | 50.566 | 31.221 | 1.00 | 0.00 | B |
| | ATOM | 3380 | CA | GLU | 302 | 24.655 | 51.931 | 29.759 | 1.00 | 19.52 | B |
| 15 | ATOM | 3381 | CB | GLU | 302 | 23.316 | 51.173 | 29.825 | 1.00 | 23.59 | B |
| | ATOM | 3382 | CG | GLU | 302 | 22.069 | 51.902 | 29.281 | 1.00 | 26.77 | B |
| | ATOM | 3383 | CD | GLU | 302 | 20.820 | 51.024 | 29.367 | 1.00 | 19.66 | B |
| | ATOM | 3384 | OE1 | GLU | 302 | 20.836 | 49.919 | 28.798 | 1.00 | 15.94 | B |
| | ATOM | 3385 | OE2 | GLU | 302 | 19.836 | 51.428 | 30.010 | 1.00 | 19.29 | B |
| 20 | ATOM | 3386 | C | GLU | 302 | 24.487 | 53.409 | 30.163 | 1.00 | 13.52 | B |
| | ATOM | 3387 | O | GLU | 302 | 24.426 | 54.276 | 29.303 | 1.00 | 17.34 | B |
| | ATOM | 3388 | N | ILE | 303 | 24.419 | 53.710 | 31.452 | 1.00 | 17.66 | B |
| | ATOM | 3389 | H | ILE | 303 | 24.459 | 53.009 | 32.135 | 1.00 | 0.00 | B |
| | ATOM | 3390 | CA | ILE | 303 | 24.282 | 55.117 | 31.825 | 1.00 | 15.73 | B |
| 25 | ATOM | 3391 | CB | ILE | 303 | 24.030 | 55.310 | 33.330 | 1.00 | 18.32 | B |
| | ATOM | 3392 | CG2 | ILE | 303 | 23.348 | 56.686 | 33.566 | 1.00 | 12.98 | B |
| | ATOM | 3393 | CG1 | ILE | 303 | 23.163 | 54.164 | 33.864 | 1.00 | 21.47 | B |
| | ATOM | 3394 | CD1 | ILE | 303 | 21.731 | 54.137 | 33.322 | 1.00 | 24.44 | B |
| | ATOM | 3395 | C | ILE | 303 | 25.575 | 55.848 | 31.452 | 1.00 | 20.62 | B |
| 30 | ATOM | 3396 | O | ILE | 303 | 25.542 | 57.005 | 31.051 | 1.00 | 22.42 | B |
| | ATOM | 3397 | N | LYS | 304 | 26.715 | 55.172 | 31.593 | 1.00 | 17.68 | B |
| | ATOM | 3398 | H | LYS | 304 | 26.703 | 54.253 | 31.932 | 1.00 | 0.00 | B |
| | ATOM | 3399 | CA | LYS | 304 | 27.980 | 55.805 | 31.236 | 1.00 | 22.51 | B |
| | ATOM | 3400 | CB | LYS | 304 | 29.183 | 54.907 | 31.567 | 1.00 | 13.79 | B |
| 35 | ATOM | 3401 | CG | LYS | 304 | 30.528 | 55.611 | 31.424 | 1.00 | 27.58 | B |
| | ATOM | 3402 | CD | LYS | 304 | 31.449 | 55.355 | 32.617 | 1.00 | 29.45 | B |
| | ATOM | 3403 | CE | LYS | 304 | 32.745 | 56.172 | 32.533 | 1.00 | 33.25 | B |
| | ATOM | 3404 | NZ | LYS | 304 | 33.272 | 56.638 | 33.870 | 1.00 | 32.84 | B |
| | ATOM | 3405 | HZ1 | LYS | 304 | 33.470 | 55.816 | 34.473 | 1.00 | 0.00 | B |
| 40 | ATOM | 3406 | HZ2 | LYS | 304 | 32.561 | 57.243 | 34.330 | 1.00 | 0.00 | B |
| | ATOM | 3407 | HZ3 | LYS | 304 | 34.147 | 57.184 | 33.727 | 1.00 | 0.00 | B |
| | ATOM | 3408 | C | LYS | 304 | 27.963 | 56.096 | 29.745 | 1.00 | 20.33 | B |
| | ATOM | 3409 | O | LYS | 304 | 28.455 | 57.130 | 29.307 | 1.00 | 21.96 | B |
| | ATOM | 3410 | N | SER | 305 | 27.376 | 55.185 | 28.977 | 1.00 | 16.80 | B |
| 45 | ATOM | 3411 | H | SER | 305 | 26.990 | 54.387 | 29.393 | 1.00 | 0.00 | B |
| | ATOM | 3412 | CA | SER | 305 | 27.295 | 55.346 | 27.534 | 1.00 | 20.13 | B |
| | ATOM | 3413 | CB | SER | 305 | 26.662 | 54.112 | 26.898 | 1.00 | 18.58 | B |
| | ATOM | 3414 | OG | SER | 305 | 25.453 | 54.454 | 26.253 | 1.00 | 30.77 | B |
| | ATOM | 3415 | HG | SER | 305 | 25.630 | 55.103 | 25.567 | 1.00 | 0.00 | B |
| 50 | ATOM | 3416 | C | SER | 305 | 26.517 | 56.584 | 27.107 | 1.00 | 15.70 | B |
| | ATOM | 3417 | O | SER | 305 | 26.679 | 57.045 | 25.991 | 1.00 | 14.73 | B |
| | ATOM | 3418 | N | ILE | 306 | 25.677 | 57.110 | 27.994 | 1.00 | 20.28 | B |
| | ATOM | 3419 | H | ILE | 306 | 25.593 | 56.689 | 28.877 | 1.00 | 0.00 | B |
| | ATOM | 3420 | CA | ILE | 306 | 24.872 | 58.299 | 27.698 | 1.00 | 14.20 | B |
| 55 | ATOM | 3421 | CB | ILE | 306 | 23.555 | 58.269 | 28.527 | 1.00 | 25.18 | B |
| | ATOM | 3422 | CG2 | ILE | 306 | 22.895 | 59.661 | 28.591 | 1.00 | 18.61 | B |
| | ATOM | 3423 | CG1 | ILE | 306 | 22.588 | 57.265 | 27.900 | 1.00 | 23.41 | B |
| | ATOM | 3424 | CD1 | ILE | 306 | 22.204 | 56.151 | 28.834 | 1.00 | 19.11 | B |
| | ATOM | 3425 | C | ILE | 306 | 25.656 | 59.594 | 27.985 | 1.00 | 18.43 | B |
| 60 | ATOM | 3426 | O | ILE | 306 | 25.481 | 60.596 | 27.301 | 1.00 | 15.22 | B |
| | ATOM | 3427 | N | ALA | 307 | 26.522 | 59.555 | 28.996 | 1.00 | 20.05 | B |
| | ATOM | 3428 | H | ALA | 307 | 26.607 | 58.727 | 29.512 | 1.00 | 0.00 | B |
| | ATOM | 3429 | CA | ALA | 307 | 27.350 | 60.711 | 29.369 | 1.00 | 21.87 | B |
| | ATOM | 3430 | CB | ALA | 307 | 28.291 | 60.341 | 30.515 | 1.00 | 13.67 | B |
| 65 | ATOM | 3431 | C | ALA | 307 | 28.177 | 61.271 | 28.226 | 1.00 | 15.95 | B |
| | ATOM | 3432 | O | ALA | 307 | 28.653 | 60.542 | 27.370 | 1.00 | 18.44 | B |
| | ATOM | 3433 | N | SER | 308 | 28.343 | 62.583 | 28.231 | 1.00 | 18.17 | B |
| | ATOM | 3434 | H | SER | 308 | 27.907 | 63.117 | 28.925 | 1.00 | 0.00 | B |
| | ATOM | 3435 | CA | SER | 308 | 29.154 | 63.252 | 27.225 | 1.00 | 19.58 | B |
| 70 | ATOM | 3436 | CB | SER | 308 | 28.962 | 64.759 | 27.306 | 1.00 | 15.23 | B |
| | ATOM | 3437 | OG | SER | 308 | 27.810 | 65.168 | 26.610 | 1.00 | 22.22 | B |
| | ATOM | 3438 | HG | SER | 308 | 27.890 | 64.920 | 25.685 | 1.00 | 0.00 | B |
| | ATOM | 3439 | C | SER | 308 | 30.606 | 62.935 | 27.556 | 1.00 | 16.69 | B |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 3440 | O | SER | 308 | 30.930 | 62.608 | 28.691 | 1.00 | 19.32 | B |
| | ATOM | 3441 | N | GLU | 309 | 31.478 | 63.027 | 26.570 | 1.00 | 19.87 | B |
| | ATOM | 3442 | H | GLU | 309 | 31.181 | 63.264 | 25.667 | 1.00 | 0.00 | B |
| | ATOM | 3443 | CA | GLU | 309 | 32.883 | 62.772 | 26.840 | 1.00 | 27.15 | B |
| | ATOM | 3444 | CB | GLU | 309 | 33.576 | 62.254 | 25.586 | 1.00 | 30.43 | B |
| | ATOM | 3445 | CG | GLU | 309 | 33.735 | 60.743 | 25.594 | 1.00 | 42.04 | B |
| 10 | ATOM | 3446 | CD | GLU | 309 | 33.305 | 60.100 | 24.293 | 1.00 | 51.38 | B |
| | ATOM | 3447 | OE1 | GLU | 309 | 33.438 | 58.860 | 24.165 | 1.00 | 53.41 | B |
| | ATOM | 3448 | OE2 | GLU | 309 | 32.836 | 60.835 | 23.398 | 1.00 | 53.07 | B |
| | ATOM | 3449 | C | GLU | 309 | 33.549 | 64.049 | 27.339 | 1.00 | 23.13 | B |
| | ATOM | 3450 | O | GLU | 309 | 33.260 | 65.147 | 26.859 | 1.00 | 24.83 | B |
| | ATOM | 3451 | N | PRO | 310 | 34.429 | 63.934 | 28.339 | 1.00 | 22.49 | B |
| 15 | ATOM | 3452 | CD | PRO | 310 | 35.090 | 65.153 | 28.838 | 1.00 | 22.94 | B |
| | ATOM | 3453 | CA | PRO | 310 | 34.873 | 62.730 | 29.061 | 1.00 | 20.46 | B |
| | ATOM | 3454 | CB | PRO | 310 | 36.043 | 63.238 | 29.899 | 1.00 | 21.98 | B |
| | ATOM | 3455 | CG | PRO | 310 | 35.744 | 64.692 | 30.108 | 1.00 | 22.65 | B |
| | ATOM | 3456 | C | PRO | 310 | 33.789 | 62.122 | 29.952 | 1.00 | 20.72 | B |
| | ATOM | 3457 | O | PRO | 310 | 33.170 | 62.840 | 30.748 | 1.00 | 21.32 | B |
| 20 | ATOM | 3458 | N | THR | 311 | 33.557 | 60.813 | 29.833 | 1.00 | 16.53 | B |
| | ATOM | 3459 | H | THR | 311 | 34.066 | 60.282 | 29.184 | 1.00 | 0.00 | B |
| | ATOM | 3460 | CA | THR | 311 | 32.556 | 60.172 | 30.669 | 1.00 | 20.30 | B |
| | ATOM | 3461 | CB | THR | 311 | 32.387 | 58.671 | 30.367 | 1.00 | 26.73 | B |
| | ATOM | 3462 | OG1 | THR | 311 | 33.656 | 58.018 | 30.481 | 1.00 | 33.48 | B |
| | ATOM | 3463 | HG1 | THR | 311 | 33.997 | 58.128 | 31.371 | 1.00 | 0.00 | B |
| 25 | ATOM | 3464 | CG2 | THR | 311 | 31.798 | 58.449 | 28.983 | 1.00 | 27.71 | B |
| | ATOM | 3465 | C | THR | 311 | 32.894 | 60.277 | 32.153 | 1.00 | 25.27 | B |
| | ATOM | 3466 | O | THR | 311 | 32.022 | 60.561 | 32.960 | 1.00 | 29.95 | B |
| | ATOM | 3467 | N | GLU | 312 | 34.153 | 60.052 | 32.524 | 1.00 | 24.13 | B |
| | ATOM | 3468 | H | GLU | 312 | 34.837 | 59.854 | 31.852 | 1.00 | 0.00 | B |
| | ATOM | 3469 | CA | GLU | 312 | 34.509 | 60.104 | 33.940 | 1.00 | 27.24 | B |
| 30 | ATOM | 3470 | CB | GLU | 312 | 36.004 | 59.840 | 34.153 | 1.00 | 30.20 | B |
| | ATOM | 3471 | CG | GLU | 312 | 36.889 | 60.121 | 32.953 | 1.00 | 44.57 | B |
| | ATOM | 3472 | CD | GLU | 312 | 36.932 | 58.966 | 31.967 | 1.00 | 42.06 | B |
| | ATOM | 3473 | OE1 | GLU | 312 | 37.286 | 57.844 | 32.376 | 1.00 | 44.27 | B |
| | ATOM | 3474 | OE2 | GLU | 312 | 36.609 | 59.188 | 30.778 | 1.00 | 45.67 | B |
| | ATOM | 3475 | C | GLU | 312 | 34.116 | 61.425 | 34.590 | 1.00 | 28.79 | B |
| 35 | ATOM | 3476 | O | GLU | 312 | 33.898 | 61.483 | 35.803 | 1.00 | 25.09 | B |
| | ATOM | 3477 | N | LYS | 313 | 34.028 | 62.485 | 33.795 | 1.00 | 26.01 | B |
| | ATOM | 3478 | H | LYS | 313 | 34.229 | 62.399 | 32.840 | 1.00 | 0.00 | B |
| | ATOM | 3479 | CA | LYS | 313 | 33.635 | 63.776 | 34.340 | 1.00 | 24.40 | B |
| | ATOM | 3480 | CB | LYS | 313 | 34.311 | 64.904 | 33.563 | 1.00 | 29.52 | B |
| | ATOM | 3481 | CG | LYS | 313 | 35.760 | 65.150 | 33.989 | 1.00 | 40.92 | B |
| 40 | ATOM | 3482 | CD | LYS | 313 | 35.838 | 66.011 | 35.246 | 1.00 | 42.61 | B |
| | ATOM | 3483 | CE | LYS | 313 | 37.263 | 66.454 | 35.516 | 1.00 | 44.08 | B |
| | ATOM | 3484 | NZ | LYS | 313 | 37.340 | 67.390 | 36.668 | 1.00 | 45.93 | B |
| | ATOM | 3485 | HZ1 | LYS | 313 | 36.977 | 66.918 | 37.522 | 1.00 | 0.00 | B |
| | ATOM | 3486 | HZ2 | LYS | 313 | 36.767 | 68.234 | 36.469 | 1.00 | 0.00 | B |
| | ATOM | 3487 | HZ3 | LYS | 313 | 38.329 | 67.670 | 36.822 | 1.00 | 0.00 | B |
| 45 | ATOM | 3488 | C | LYS | 313 | 32.114 | 63.968 | 34.305 | 1.00 | 23.67 | B |
| | ATOM | 3489 | O | LYS | 313 | 31.546 | 64.615 | 35.183 | 1.00 | 21.16 | B |
| | ATOM | 3490 | N | HIS | 314 | 31.462 | 63.394 | 33.299 | 1.00 | 17.77 | B |
| | ATOM | 3491 | H | HIS | 314 | 31.956 | 62.860 | 32.643 | 1.00 | 0.00 | B |
| | ATOM | 3492 | CA | HIS | 314 | 30.026 | 63.546 | 33.163 | 1.00 | 23.14 | B |
| | ATOM | 3493 | CB | HIS | 314 | 29.664 | 63.688 | 31.681 | 1.00 | 23.44 | B |
| 50 | ATOM | 3494 | CG | HIS | 314 | 30.242 | 64.916 | 31.035 | 1.00 | 26.47 | B |
| | ATOM | 3495 | CD2 | HIS | 314 | 31.317 | 65.073 | 30.226 | 1.00 | 24.55 | B |
| | ATOM | 3496 | ND1 | HIS | 314 | 29.652 | 66.157 | 31.136 | 1.00 | 27.43 | B |
| | ATOM | 3497 | HD1 | HIS | 314 | 28.867 | 66.359 | 31.682 | 1.00 | 0.00 | B |
| | ATOM | 3498 | CE1 | HIS | 314 | 30.344 | 67.031 | 30.426 | 1.00 | 13.83 | B |
| | ATOM | 3499 | NE2 | HIS | 314 | 31.355 | 66.398 | 29.864 | 1.00 | 30.72 | B |
| 55 | ATOM | 3500 | HE2 | HIS | 314 | 32.021 | 66.817 | 29.289 | 1.00 | 0.00 | B |
| | ATOM | 3501 | C | HIS | 314 | 29.178 | 62.430 | 33.812 | 1.00 | 19.97 | B |
| | ATOM | 3502 | O | HIS | 314 | 28.022 | 62.663 | 34.133 | 1.00 | 15.17 | B |
| | ATOM | 3503 | N | PHE | 315 | 29.752 | 61.245 | 34.019 | 1.00 | 12.58 | B |
| | ATOM | 3504 | H | PHE | 315 | 30.680 | 61.109 | 33.753 | 1.00 | 0.00 | B |
| | ATOM | 3505 | CA | PHE | 315 | 29.018 | 60.139 | 34.637 | 1.00 | 11.72 | B |
| 60 | ATOM | 3506 | CB | PHE | 315 | 29.435 | 58.799 | 34.022 | 1.00 | 13.63 | B |
| | ATOM | 3507 | CG | PHE | 315 | 28.821 | 57.595 | 34.702 | 1.00 | 17.15 | B |
| | ATOM | 3508 | CD1 | PHE | 315 | 27.427 | 57.409 | 34.716 | 1.00 | 12.18 | B |
| | ATOM | 3509 | CD2 | PHE | 315 | 29.626 | 56.635 | 35.320 | 1.00 | 21.49 | B |
| | ATOM | 3510 | CE1 | PHE | 315 | 26.856 | 56.290 | 35.330 | 1.00 | 15.00 | B |
| | ATOM | 3511 | CE2 | PHE | 315 | 29.052 | 55.501 | 35.941 | 1.00 | 19.73 | B |
| 65 | ATOM | 3512 | CZ | PHE | 315 | 27.651 | 55.337 | 35.943 | 1.00 | 11.10 | B |

| | | | | | | | | | | | |
|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| | ATOM | 3513 | C | PHE | 315 | 29.189 | 60.045 | 36.153 | 1.00 | 20.36 | B |
| | ATOM | 3514 | O | PHE | 315 | 30.307 | 60.141 | 36.672 | 1.00 | 18.84 | B |
| | ATOM | 3515 | N | PHE | 316 | 28.074 | 59.844 | 36.863 | 1.00 | 23.38 | B |
| | ATOM | 3516 | H | PHE | 316 | 27.214 | 59.795 | 36.398 | 1.00 | 0.00 | B |
| 5 | ATOM | 3517 | CA | PHE | 316 | 28.107 | 59.697 | 38.317 | 1.00 | 14.23 | B |
| | ATOM | 3518 | CB | PHE | 316 | 27.395 | 60.853 | 39.002 | 1.00 | 19.22 | B |
| | ATOM | 3519 | CG | PHE | 316 | 28.065 | 62.188 | 38.810 | 1.00 | 27.88 | B |
| | ATOM | 3520 | CD1 | PHE | 316 | 27.744 | 62.994 | 37.721 | 1.00 | 28.03 | B |
| 10 | ATOM | 3521 | CD2 | PHE | 316 | 28.969 | 62.675 | 39.754 | 1.00 | 31.78 | B |
| | ATOM | 3522 | CE1 | PHE | 316 | 28.306 | 64.271 | 37.578 | 1.00 | 29.90 | B |
| | ATOM | 3523 | CE2 | PHE | 316 | 29.535 | 63.959 | 39.609 | 1.00 | 25.22 | B |
| | ATOM | 3524 | CZ | PHE | 316 | 29.195 | 64.746 | 38.523 | 1.00 | 25.24 | B |
| | ATOM | 3525 | C | PHE | 316 | 27.453 | 58.392 | 38.737 | 1.00 | 19.30 | B |
| | ATOM | 3526 | O | PHE | 316 | 26.306 | 58.100 | 38.370 | 1.00 | 16.18 | B |
| 15 | ATOM | 3527 | N | ASN | 317 | 28.194 | 57.593 | 39.489 | 1.00 | 22.70 | B |
| | ATOM | 3528 | H | ASN | 317 | 29.106 | 57.868 | 39.725 | 1.00 | 0.00 | B |
| | ATOM | 3529 | CA | ASN | 317 | 27.695 | 56.312 | 39.979 | 1.00 | 23.24 | B |
| | ATOM | 3530 | CB | ASN | 317 | 28.741 | 55.210 | 39.759 | 1.00 | 22.04 | B |
| | ATOM | 3531 | CG | ASN | 317 | 28.335 | 53.871 | 40.391 | 1.00 | 25.87 | B |
| 20 | ATOM | 3532 | OD1 | ASN | 317 | 27.738 | 53.828 | 41.467 | 1.00 | 26.08 | B |
| | ATOM | 3533 | ND2 | ASN | 317 | 28.658 | 52.778 | 39.716 | 1.00 | 13.17 | B |
| | ATOM | 3534 | HD21 | ASN | 317 | 29.130 | 52.855 | 38.858 | 1.00 | 0.00 | B |
| | ATOM | 3535 | HD22 | ASN | 317 | 28.407 | 51.916 | 40.103 | 1.00 | 0.00 | B |
| | ATOM | 3536 | C | ASN | 317 | 27.410 | 56.484 | 41.463 | 1.00 | 18.96 | B |
| 25 | ATOM | 3537 | O | ASN | 317 | 28.326 | 56.476 | 42.277 | 1.00 | 21.45 | B |
| | ATOM | 3538 | N | VAL | 318 | 26.142 | 56.669 | 41.804 | 1.00 | 23.81 | B |
| | ATOM | 3539 | H | VAL | 318 | 25.458 | 56.678 | 41.102 | 1.00 | 0.00 | B |
| | ATOM | 3540 | CA | VAL | 318 | 25.731 | 56.857 | 43.187 | 1.00 | 20.00 | B |
| | ATOM | 3541 | CB | VAL | 318 | 24.576 | 57.902 | 43.272 | 1.00 | 21.73 | B |
| 30 | ATOM | 3542 | CG1 | VAL | 318 | 23.466 | 57.514 | 42.335 | 1.00 | 27.34 | B |
| | ATOM | 3543 | CG2 | VAL | 318 | 24.060 | 58.012 | 44.688 | 1.00 | 15.43 | B |
| | ATOM | 3544 | C | VAL | 318 | 25.280 | 55.508 | 43.737 | 1.00 | 20.44 | B |
| | ATOM | 3545 | O | VAL | 318 | 24.488 | 54.814 | 43.108 | 1.00 | 17.67 | B |
| | ATOM | 3546 | N | SER | 319 | 25.797 | 55.133 | 44.903 | 1.00 | 20.29 | B |
| 35 | ATOM | 3547 | H | SER | 319 | 26.417 | 55.731 | 45.369 | 1.00 | 0.00 | B |
| | ATOM | 3548 | CA | SER | 319 | 25.455 | 53.840 | 45.502 | 1.00 | 17.71 | B |
| | ATOM | 3549 | CB | SER | 319 | 26.268 | 53.608 | 46.775 | 1.00 | 13.81 | B |
| | ATOM | 3550 | OG | SER | 319 | 27.123 | 54.701 | 47.038 | 1.00 | 31.29 | B |
| | ATOM | 3551 | HG | SER | 319 | 26.599 | 55.496 | 47.151 | 1.00 | 0.00 | B |
| 40 | ATOM | 3552 | C | SER | 319 | 23.969 | 53.697 | 45.816 | 1.00 | 18.64 | B |
| | ATOM | 3553 | O | SER | 319 | 23.382 | 52.644 | 45.575 | 1.00 | 16.85 | B |
| | ATOM | 3554 | N | ASP | 320 | 23.361 | 54.745 | 46.351 | 1.00 | 16.38 | B |
| | ATOM | 3555 | H | ASP | 320 | 23.866 | 55.566 | 46.537 | 1.00 | 0.00 | B |
| | ATOM | 3556 | CA | ASP | 320 | 21.943 | 54.679 | 46.665 | 1.00 | 20.08 | B |
| 45 | ATOM | 3557 | CB | ASP | 320 | 21.720 | 53.772 | 47.878 | 1.00 | 26.71 | B |
| | ATOM | 3558 | CG | ASP | 320 | 22.310 | 54.337 | 49.143 | 1.00 | 23.52 | B |
| | ATOM | 3559 | OD1 | ASP | 320 | 23.287 | 55.104 | 49.059 | 1.00 | 27.09 | B |
| | ATOM | 3560 | OD2 | ASP | 320 | 21.791 | 54.013 | 50.227 | 1.00 | 27.50 | B |
| | ATOM | 3561 | C | ASP | 320 | 21.317 | 56.062 | 46.886 | 1.00 | 16.45 | B |
| 50 | ATOM | 3562 | O | ASP | 320 | 22.018 | 57.062 | 47.037 | 1.00 | 15.80 | B |
| | ATOM | 3563 | N | GLU | 321 | 19.991 | 56.088 | 46.902 | 1.00 | 14.19 | B |
| | ATOM | 3564 | H | GLU | 321 | 19.508 | 55.238 | 46.818 | 1.00 | 0.00 | B |
| | ATOM | 3565 | CA | GLU | 321 | 19.220 | 57.313 | 47.037 | 1.00 | 21.02 | B |
| | ATOM | 3566 | CB | GLU | 321 | 17.738 | 56.966 | 47.233 | 1.00 | 12.70 | B |
| 55 | ATOM | 3567 | CG | GLU | 321 | 17.115 | 56.285 | 46.017 | 1.00 | 12.53 | B |
| | ATOM | 3568 | CD | GLU | 321 | 17.187 | 54.767 | 46.098 | 1.00 | 17.82 | B |
| | ATOM | 3569 | OE1 | GLU | 321 | 17.982 | 54.231 | 46.903 | 1.00 | 14.77 | B |
| | ATOM | 3570 | OE2 | GLU | 321 | 16.439 | 54.103 | 45.355 | 1.00 | 17.04 | B |
| | ATOM | 3571 | C | GLU | 321 | 19.675 | 58.272 | 48.130 | 1.00 | 24.90 | B |
| 60 | ATOM | 3572 | O | GLU | 321 | 19.749 | 59.480 | 47.906 | 1.00 | 22.58 | B |
| | ATOM | 3573 | N | LEU | 322 | 19.967 | 57.732 | 49.307 | 1.00 | 26.45 | B |
| | ATOM | 3574 | H | LEU | 322 | 19.881 | 56.763 | 49.428 | 1.00 | 0.00 | B |
| | ATOM | 3575 | CA | LEU | 322 | 20.411 | 58.550 | 50.425 | 1.00 | 28.16 | B |
| | ATOM | 3576 | CB | LEU | 322 | 20.477 | 57.707 | 51.709 | 1.00 | 32.06 | B |
| 65 | ATOM | 3577 | CG | LEU | 322 | 19.155 | 57.600 | 52.478 | 1.00 | 34.11 | B |
| | ATOM | 3578 | CD1 | LEU | 322 | 19.357 | 56.923 | 53.839 | 1.00 | 29.26 | B |
| | ATOM | 3579 | CD2 | LEU | 322 | 18.583 | 59.000 | 52.645 | 1.00 | 30.30 | B |
| | ATOM | 3580 | C | LEU | 322 | 21.768 | 59.193 | 50.154 | 1.00 | 30.66 | B |
| | ATOM | 3581 | O | LEU | 322 | 22.119 | 60.195 | 50.776 | 1.00 | 33.88 | B |
| 70 | ATOM | 3582 | N | ALA | 323 | 22.527 | 58.625 | 49.219 | 1.00 | 26.52 | B |
| | ATOM | 3583 | H | ALA | 323 | 22.199 | 57.828 | 48.752 | 1.00 | 0.00 | B |
| | ATOM | 3584 | CA | ALA | 323 | 23.839 | 59.166 | 48.886 | 1.00 | 24.47 | B |
| | ATOM | 3585 | CB | ALA | 323 | 24.772 | 58.030 | 48.451 | 1.00 | 19.17 | B |

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|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 3586 | C | ALA | 323 | 23.832 | 60.283 | 47.820 | 1.00 | 24.00 | B |
| | ATOM | 3587 | O | ALA | 323 | 24.829 | 60.971 | 47.657 | 1.00 | 24.66 | B |
| | ATOM | 3588 | N | LEU | 324 | 22.735 | 60.481 | 47.096 | 1.00 | 21.81 | B |
| | ATOM | 3589 | H | LEU | 324 | 21.941 | 59.928 | 47.248 | 1.00 | 0.00 | B |
| | ATOM | 3590 | CA | LEU | 324 | 22.715 | 61.534 | 46.069 | 1.00 | 19.68 | B |
| 10 | ATOM | 3591 | CB | LEU | 324 | 21.312 | 61.715 | 45.508 | 1.00 | 18.39 | B |
| | ATOM | 3592 | CG | LEU | 324 | 20.899 | 60.637 | 44.519 | 1.00 | 13.78 | B |
| | ATOM | 3593 | CD1 | LEU | 324 | 19.402 | 60.611 | 44.457 | 1.00 | 16.65 | B |
| | ATOM | 3594 | CD2 | LEU | 324 | 21.511 | 60.908 | 43.143 | 1.00 | 14.31 | B |
| | ATOM | 3595 | C | LEU | 324 | 23.226 | 62.892 | 46.561 | 1.00 | 23.65 | B |
| 15 | ATOM | 3596 | O | LEU | 324 | 23.938 | 63.594 | 45.841 | 1.00 | 18.23 | B |
| | ATOM | 3597 | N | VAL | 325 | 22.852 | 63.264 | 47.783 | 1.00 | 26.30 | B |
| | ATOM | 3598 | H | VAL | 325 | 22.272 | 62.672 | 48.305 | 1.00 | 0.00 | B |
| | ATOM | 3599 | CA | VAL | 325 | 23.282 | 64.533 | 48.369 | 1.00 | 31.91 | B |
| | ATOM | 3600 | CB | VAL | 325 | 22.778 | 64.643 | 49.837 | 1.00 | 37.44 | B |
| 20 | ATOM | 3601 | CG1 | VAL | 325 | 23.583 | 65.687 | 50.609 | 1.00 | 34.83 | B |
| | ATOM | 3602 | CG2 | VAL | 325 | 21.294 | 65.008 | 49.843 | 1.00 | 42.56 | B |
| | ATOM | 3603 | C | VAL | 325 | 24.819 | 64.710 | 48.330 | 1.00 | 30.26 | B |
| | ATOM | 3604 | O | VAL | 325 | 25.327 | 65.825 | 48.398 | 1.00 | 32.04 | B |
| | ATOM | 3605 | N | THR | 326 | 25.548 | 63.609 | 48.194 | 1.00 | 28.75 | B |
| 25 | ATOM | 3606 | H | THR | 326 | 25.094 | 62.744 | 48.113 | 1.00 | 0.00 | B |
| | ATOM | 3607 | CA | THR | 326 | 26.998 | 63.657 | 48.167 | 1.00 | 31.17 | B |
| | ATOM | 3608 | CB | THR | 326 | 27.607 | 62.288 | 48.511 | 1.00 | 27.84 | B |
| | ATOM | 3609 | OG1 | THR | 326 | 27.229 | 61.332 | 47.514 | 1.00 | 34.82 | B |
| | ATOM | 3610 | HG1 | THR | 326 | 26.277 | 61.260 | 47.489 | 1.00 | 0.00 | B |
| 30 | ATOM | 3611 | CG2 | THR | 326 | 27.136 | 61.826 | 49.880 | 1.00 | 30.51 | B |
| | ATOM | 3612 | C | THR | 326 | 27.608 | 64.128 | 46.856 | 1.00 | 32.05 | B |
| | ATOM | 3613 | O | THR | 326 | 28.745 | 64.590 | 46.846 | 1.00 | 30.58 | B |
| | ATOM | 3614 | N | ILE | 327 | 26.879 | 64.002 | 45.750 | 1.00 | 33.07 | B |
| | ATOM | 3615 | H | ILE | 327 | 25.984 | 63.603 | 45.793 | 1.00 | 0.00 | B |
| 35 | ATOM | 3616 | CA | ILE | 327 | 27.421 | 64.461 | 44.472 | 1.00 | 32.83 | B |
| | ATOM | 3617 | CB | ILE | 327 | 27.185 | 63.446 | 43.300 | 1.00 | 35.01 | B |
| | ATOM | 3618 | CG2 | ILE | 327 | 27.881 | 62.118 | 43.604 | 1.00 | 32.57 | B |
| | ATOM | 3619 | CG1 | ILE | 327 | 25.691 | 63.252 | 43.048 | 1.00 | 35.05 | B |
| | ATOM | 3620 | CD1 | ILE | 327 | 25.371 | 62.796 | 41.633 | 1.00 | 32.92 | B |
| 40 | ATOM | 3621 | C | ILE | 327 | 26.852 | 65.814 | 44.061 | 1.00 | 30.01 | B |
| | ATOM | 3622 | O | ILE | 327 | 27.211 | 66.348 | 43.011 | 1.00 | 23.73 | B |
| | ATOM | 3623 | N | VAL | 328 | 25.972 | 66.370 | 44.894 | 1.00 | 26.90 | B |
| | ATOM | 3624 | H | VAL | 328 | 25.715 | 65.896 | 45.711 | 1.00 | 0.00 | B |
| | ATOM | 3625 | CA | VAL | 328 | 25.383 | 67.675 | 44.600 | 1.00 | 32.68 | B |
| 45 | ATOM | 3626 | CB | VAL | 328 | 24.535 | 68.177 | 45.798 | 1.00 | 36.74 | B |
| | ATOM | 3627 | CG1 | VAL | 328 | 24.075 | 69.612 | 45.561 | 1.00 | 29.92 | B |
| | ATOM | 3628 | CG2 | VAL | 328 | 23.332 | 67.265 | 45.998 | 1.00 | 30.30 | B |
| | ATOM | 3629 | C | VAL | 328 | 26.451 | 68.741 | 44.255 | 1.00 | 33.15 | B |
| | ATOM | 3630 | O | VAL | 328 | 26.310 | 69.477 | 43.279 | 1.00 | 35.10 | B |
| 50 | ATOM | 3631 | N | LYS | 329 | 27.528 | 68.801 | 45.038 | 1.00 | 32.80 | B |
| | ATOM | 3632 | H | LYS | 329 | 27.613 | 68.169 | 45.781 | 1.00 | 0.00 | B |
| | ATOM | 3633 | CA | LYS | 329 | 28.585 | 69.789 | 44.819 | 1.00 | 31.42 | B |
| | ATOM | 3634 | CB | LYS | 329 | 29.563 | 69.773 | 45.990 | 1.00 | 38.34 | B |
| | ATOM | 3635 | CG | LYS | 329 | 29.794 | 71.139 | 46.623 | 1.00 | 42.75 | B |
| 55 | ATOM | 3636 | CD | LYS | 329 | 29.245 | 71.201 | 48.053 | 1.00 | 46.58 | B |
| | ATOM | 3637 | CE | LYS | 329 | 27.716 | 71.275 | 48.078 | 1.00 | 48.13 | B |
| | ATOM | 3638 | NZ | LYS | 329 | 27.089 | 70.078 | 48.711 | 1.00 | 48.31 | B |
| | ATOM | 3639 | HZ1 | LYS | 329 | 27.420 | 69.992 | 49.693 | 1.00 | 0.00 | B |
| | ATOM | 3640 | HZ2 | LYS | 329 | 27.357 | 69.225 | 48.180 | 1.00 | 0.00 | B |
| 60 | ATOM | 3641 | HZ3 | LYS | 329 | 26.055 | 70.182 | 48.701 | 1.00 | 0.00 | B |
| | ATOM | 3642 | C | LYS | 329 | 29.365 | 69.648 | 43.517 | 1.00 | 29.75 | B |
| | ATOM | 3643 | O | LYS | 329 | 29.548 | 70.633 | 42.791 | 1.00 | 30.62 | B |
| | ATOM | 3644 | N | ALA | 330 | 29.818 | 68.434 | 43.226 | 1.00 | 27.05 | B |
| | ATOM | 3645 | H | ALA | 330 | 29.623 | 67.699 | 43.844 | 1.00 | 0.00 | B |
| 65 | ATOM | 3646 | CA | ALA | 330 | 30.598 | 68.145 | 42.022 | 1.00 | 27.52 | B |
| | ATOM | 3647 | CB | ALA | 330 | 31.094 | 66.683 | 42.058 | 1.00 | 15.14 | B |
| | ATOM | 3648 | C | ALA | 330 | 29.804 | 68.397 | 40.742 | 1.00 | 24.45 | B |
| | ATOM | 3649 | O | ALA | 330 | 30.282 | 69.043 | 39.811 | 1.00 | 29.53 | B |
| | ATOM | 3650 | N | LEU | 331 | 28.585 | 67.878 | 40.708 | 1.00 | 27.74 | B |
| 70 | ATOM | 3651 | H | LEU | 331 | 28.266 | 67.372 | 41.483 | 1.00 | 0.00 | B |
| | ATOM | 3652 | CA | LEU | 331 | 27.701 | 68.040 | 39.555 | 1.00 | 26.77 | B |
| | ATOM | 3653 | CB | LEU | 331 | 26.398 | 67.267 | 39.771 | 1.00 | 20.69 | B |
| | ATOM | 3654 | CG | LEU | 331 | 25.594 | 66.834 | 38.543 | 1.00 | 27.56 | B |
| | ATOM | 3655 | CD1 | LEU | 331 | 24.126 | 67.117 | 38.817 | 1.00 | 32.10 | B |
| | ATOM | 3656 | CD2 | LEU | 331 | 26.079 | 67.540 | 37.280 | 1.00 | 22.24 | B |
| | ATOM | 3657 | C | LEU | 331 | 27.358 | 69.497 | 39.326 | 1.00 | 14.45 | B |
| | ATOM | 3658 | O | LEU | 331 | 27.376 | 69.973 | 38.209 | 1.00 | 25.05 | B |

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|----|------|------|------|-----|-----|--------|--------|--------|------|-------|---|
| | ATOM | 3659 | N | GLY | 332 | 27.036 | 70.199 | 40.400 | 1.00 | 20.98 | B |
| | ATOM | 3660 | H | GLY | 332 | 27.036 | 69.772 | 41.280 | 1.00 | 0.00 | B |
| | ATOM | 3661 | CA | GLY | 332 | 26.683 | 71.599 | 40.277 | 1.00 | 16.97 | B |
| 5 | ATOM | 3662 | C | GLY | 332 | 27.830 | 72.431 | 39.740 | 1.00 | 23.19 | B |
| | ATOM | 3663 | O | GLY | 332 | 27.611 | 73.389 | 39.000 | 1.00 | 20.06 | B |
| | ATOM | 3664 | N | GLU | 333 | 29.063 | 72.086 | 40.102 | 1.00 | 22.14 | B |
| | ATOM | 3665 | H | GLU | 333 | 29.218 | 71.324 | 40.699 | 1.00 | 0.00 | B |
| | ATOM | 3666 | CA | GLU | 333 | 30.169 | 72.870 | 39.589 | 1.00 | 28.24 | B |
| 10 | ATOM | 3667 | CB | GLU | 333 | 31.358 | 72.859 | 40.557 | 1.00 | 33.30 | B |
| | ATOM | 3668 | CG | GLU | 333 | 31.779 | 71.505 | 41.068 | 1.00 | 40.29 | B |
| | ATOM | 3669 | CD | GLU | 333 | 33.065 | 71.595 | 41.866 | 1.00 | 46.24 | B |
| | ATOM | 3670 | OE1 | GLU | 333 | 34.122 | 71.152 | 41.350 | 1.00 | 45.00 | B |
| | ATOM | 3671 | OE2 | GLU | 333 | 33.008 | 72.121 | 43.006 | 1.00 | 38.74 | B |
| | ATOM | 3672 | C | GLU | 333 | 30.594 | 72.407 | 38.206 | 1.00 | 27.85 | B |
| 15 | ATOM | 3673 | O | GLU | 333 | 31.048 | 73.215 | 37.397 | 1.00 | 29.71 | B |
| | ATOM | 3674 | N | ARG | 334 | 30.438 | 71.115 | 37.920 | 1.00 | 25.03 | B |
| | ATOM | 3675 | H | ARG | 334 | 30.079 | 70.508 | 38.601 | 1.00 | 0.00 | B |
| | ATOM | 3676 | CA | ARG | 334 | 30.799 | 70.594 | 36.602 | 1.00 | 18.82 | B |
| 20 | ATOM | 3677 | CB | ARG | 334 | 30.839 | 69.062 | 36.610 | 1.00 | 17.45 | B |
| | ATOM | 3678 | CG | ARG | 334 | 32.187 | 68.485 | 36.951 | 1.00 | 12.28 | B |
| | ATOM | 3679 | CD | ARG | 334 | 32.112 | 66.986 | 37.157 | 1.00 | 20.12 | B |
| | ATOM | 3680 | NE | ARG | 334 | 33.151 | 66.520 | 38.065 | 1.00 | 26.33 | B |
| | ATOM | 3681 | HE | ARG | 334 | 33.835 | 67.163 | 38.343 | 1.00 | 0.00 | B |
| | ATOM | 3682 | CZ | ARG | 334 | 33.230 | 65.281 | 38.543 | 1.00 | 33.67 | B |
| 25 | ATOM | 3683 | NH1 | ARG | 334 | 32.321 | 64.366 | 38.200 | 1.00 | 28.50 | B |
| | ATOM | 3684 | HH11 | ARG | 334 | 31.575 | 64.611 | 37.583 | 1.00 | 0.00 | B |
| | ATOM | 3685 | HH12 | ARG | 334 | 32.388 | 63.437 | 38.563 | 1.00 | 0.00 | B |
| | ATOM | 3686 | NH2 | ARG | 334 | 34.220 | 64.956 | 39.364 | 1.00 | 33.01 | B |
| | ATOM | 3687 | HH21 | ARG | 334 | 34.901 | 65.642 | 39.624 | 1.00 | 0.00 | B |
| 30 | ATOM | 3688 | HH22 | ARG | 334 | 34.287 | 64.026 | 39.728 | 1.00 | 0.00 | B |
| | ATOM | 3689 | C | ARG | 334 | 29.811 | 71.057 | 35.532 | 1.00 | 16.42 | B |
| | ATOM | 3690 | O | ARG | 334 | 30.185 | 71.277 | 34.383 | 1.00 | 17.09 | B |
| | ATOM | 3691 | N | ILE | 335 | 28.541 | 71.184 | 35.889 | 1.00 | 18.26 | B |
| 35 | ATOM | 3692 | H | ILE | 335 | 28.256 | 70.974 | 36.802 | 1.00 | 0.00 | B |
| | ATOM | 3693 | CA | ILE | 335 | 27.574 | 71.640 | 34.899 | 1.00 | 21.52 | B |
| | ATOM | 3694 | CB | ILE | 335 | 26.166 | 71.818 | 35.518 | 1.00 | 22.25 | B |
| | ATOM | 3695 | CG2 | ILE | 335 | 26.288 | 72.266 | 36.946 | 1.00 | 30.01 | B |
| | ATOM | 3696 | CG1 | ILE | 335 | 25.365 | 72.886 | 34.776 | 1.00 | 13.73 | B |
| 40 | ATOM | 3697 | CD1 | ILE | 335 | 25.018 | 72.533 | 33.362 | 1.00 | 25.02 | B |
| | ATOM | 3698 | C | ILE | 335 | 28.053 | 72.976 | 34.345 | 1.00 | 24.47 | B |
| | ATOM | 3699 | O | ILE | 335 | 28.012 | 73.203 | 33.135 | 1.00 | 23.62 | B |
| | ATOM | 3700 | N | PHE | 336 | 28.537 | 73.841 | 35.235 | 1.00 | 24.00 | B |
| | ATOM | 3701 | H | PHE | 336 | 28.593 | 73.575 | 36.176 | 1.00 | 0.00 | B |
| 45 | ATOM | 3702 | CA | PHE | 336 | 28.987 | 75.179 | 34.848 | 1.00 | 29.92 | B |
| | ATOM | 3703 | CB | PHE | 336 | 28.561 | 76.179 | 35.932 | 1.00 | 31.59 | B |
| | ATOM | 3704 | CG | PHE | 336 | 27.077 | 76.412 | 35.973 | 1.00 | 26.05 | B |
| | ATOM | 3705 | CD1 | PHE | 336 | 26.290 | 75.810 | 36.955 | 1.00 | 30.05 | B |
| | ATOM | 3706 | CD2 | PHE | 336 | 26.459 | 77.184 | 34.993 | 1.00 | 24.28 | B |
| 50 | ATOM | 3707 | CE1 | PHE | 336 | 24.895 | 75.970 | 36.958 | 1.00 | 25.70 | B |
| | ATOM | 3708 | CE2 | PHE | 336 | 25.072 | 77.353 | 34.981 | 1.00 | 26.15 | B |
| | ATOM | 3709 | CZ | PHE | 336 | 24.287 | 76.738 | 35.971 | 1.00 | 22.17 | B |
| | ATOM | 3710 | C | PHE | 336 | 30.463 | 75.384 | 34.495 | 1.00 | 31.44 | B |
| | ATOM | 3711 | O | PHE | 336 | 30.870 | 76.491 | 34.124 | 1.00 | 27.91 | B |
| 55 | ATOM | 3712 | N | ALA | 337 | 31.260 | 74.328 | 34.583 | 1.00 | 30.25 | B |
| | ATOM | 3713 | H | ALA | 337 | 30.895 | 73.465 | 34.875 | 1.00 | 0.00 | B |
| | ATOM | 3714 | CA | ALA | 337 | 32.674 | 74.440 | 34.253 | 1.00 | 35.57 | B |
| | ATOM | 3715 | CB | ALA | 337 | 33.518 | 74.124 | 35.479 | 1.00 | 31.23 | B |
| | ATOM | 3716 | C | ALA | 337 | 33.085 | 73.537 | 33.083 | 1.00 | 38.16 | B |
| 60 | ATOM | 3717 | O | ALA | 337 | 33.755 | 73.989 | 32.162 | 1.00 | 40.82 | B |
| | ATOM | 3718 | N | LEU | 338 | 32.668 | 72.271 | 33.125 | 1.00 | 41.05 | B |
| | ATOM | 3719 | H | LEU | 338 | 32.114 | 71.987 | 33.880 | 1.00 | 0.00 | B |
| | ATOM | 3720 | CA | LEU | 338 | 33.003 | 71.286 | 32.092 | 1.00 | 43.90 | B |
| | ATOM | 3721 | CB | LEU | 338 | 32.334 | 69.943 | 32.405 | 1.00 | 43.75 | B |
| 65 | ATOM | 3722 | CG | LEU | 338 | 33.195 | 68.796 | 32.939 | 1.00 | 46.43 | B |
| | ATOM | 3723 | CD1 | LEU | 338 | 32.356 | 67.526 | 33.010 | 1.00 | 48.40 | B |
| | ATOM | 3724 | CD2 | LEU | 338 | 34.406 | 68.586 | 32.043 | 1.00 | 46.34 | B |
| | ATOM | 3725 | C | LEU | 338 | 32.609 | 71.712 | 30.683 | 1.00 | 47.43 | B |
| | ATOM | 3726 | O | LEU | 338 | 33.390 | 71.430 | 29.740 | 1.00 | 47.18 | B |
| 70 | ATOM | 3727 | OT | LEU | 338 | 31.518 | 72.308 | 30.541 | 1.00 | 50.73 | B |
| | ATOM | 3728 | OH2 | H2O | 1 | 11.763 | 72.942 | 27.999 | 1.00 | 13.08 | W |
| | ATOM | 3729 | H1 | H2O | 1 | 12.196 | 72.994 | 27.149 | 1.00 | 0.00 | W |
| | ATOM | 3730 | H2 | H2O | 1 | 11.929 | 72.051 | 28.302 | 1.00 | 0.00 | W |
| | ATOM | 3731 | OH2 | H2O | 2 | 33.606 | 75.805 | 28.263 | 1.00 | 38.72 | W |

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|----|------|------|-----|-----|----|--------|--------|---------|------|-------|---|
| 5 | ATOM | 3732 | H1 | H2O | 2 | 33.652 | 75.559 | 29.186 | 1.00 | 0.00 | W |
| | ATOM | 3733 | H2 | H2O | 2 | 33.674 | 76.762 | 28.267 | 1.00 | 0.00 | W |
| | ATOM | 3734 | OH2 | H2O | 3 | 46.772 | 76.583 | -1.078 | 1.00 | 59.42 | W |
| | ATOM | 3735 | H1 | H2O | 3 | 46.862 | 77.129 | -1.859 | 1.00 | 0.00 | W |
| | ATOM | 3736 | H2 | H2O | 3 | 47.663 | 76.280 | -0.894 | 1.00 | 0.00 | W |
| 10 | ATOM | 3737 | OH2 | H2O | 4 | 17.892 | 53.996 | 32.616 | 1.00 | 12.25 | W |
| | ATOM | 3738 | H1 | H2O | 4 | 17.234 | 54.300 | 31.991 | 1.00 | 0.00 | W |
| | ATOM | 3739 | H2 | H2O | 4 | 17.561 | 53.146 | 32.907 | 1.00 | 0.00 | W |
| | ATOM | 3740 | OH2 | H2O | 5 | 28.607 | 56.204 | 23.823 | 1.00 | 37.75 | W |
| | ATOM | 3741 | H1 | H2O | 5 | 27.946 | 56.312 | 24.504 | 1.00 | 0.00 | W |
| 15 | ATOM | 3742 | H2 | H2O | 5 | 29.014 | 57.067 | 23.742 | 1.00 | 0.00 | W |
| | ATOM | 3743 | OH2 | H2O | 6 | 33.273 | 78.294 | 33.342 | 1.00 | 29.21 | W |
| | ATOM | 3744 | H1 | H2O | 6 | 32.852 | 77.437 | 33.359 | 1.00 | 0.00 | W |
| | ATOM | 3745 | H2 | H2O | 6 | 32.646 | 78.878 | 33.776 | 1.00 | 0.00 | W |
| | ATOM | 3746 | OH2 | H2O | 7 | 17.238 | 53.571 | 16.889 | 1.00 | 44.25 | W |
| 20 | ATOM | 3747 | H1 | H2O | 7 | 16.904 | 53.246 | 16.055 | 1.00 | 0.00 | W |
| | ATOM | 3748 | H2 | H2O | 7 | 17.520 | 52.787 | 17.360 | 1.00 | 0.00 | W |
| | ATOM | 3749 | OH2 | H2O | 8 | 13.870 | 78.571 | 33.824 | 1.00 | 15.18 | W |
| | ATOM | 3750 | H1 | H2O | 8 | 13.855 | 78.968 | 34.695 | 1.00 | 0.00 | W |
| | ATOM | 3751 | H2 | H2O | 8 | 13.148 | 79.001 | 33.357 | 1.00 | 0.00 | W |
| 25 | ATOM | 3752 | OH2 | H2O | 9 | 25.865 | 90.956 | -20.487 | 1.00 | 31.46 | W |
| | ATOM | 3753 | H1 | H2O | 9 | 25.185 | 90.524 | -21.011 | 1.00 | 0.00 | W |
| | ATOM | 3754 | H2 | H2O | 9 | 25.994 | 90.377 | -19.740 | 1.00 | 0.00 | W |
| | ATOM | 3755 | OH2 | H2O | 10 | 36.614 | 69.921 | 37.968 | 1.00 | 47.49 | W |
| | ATOM | 3756 | H1 | H2O | 10 | 37.012 | 69.641 | 38.786 | 1.00 | 0.00 | W |
| 30 | ATOM | 3757 | H2 | H2O | 10 | 37.218 | 69.613 | 37.294 | 1.00 | 0.00 | W |
| | ATOM | 3758 | OH2 | H2O | 11 | 25.295 | 79.036 | 26.770 | 1.00 | 27.54 | W |
| | ATOM | 3759 | H1 | H2O | 11 | 24.707 | 79.474 | 26.157 | 1.00 | 0.00 | W |
| | ATOM | 3760 | H2 | H2O | 11 | 24.928 | 79.225 | 27.628 | 1.00 | 0.00 | W |
| | ATOM | 3761 | OH2 | H2O | 12 | 18.365 | 40.699 | 50.184 | 1.00 | 18.35 | W |
| 35 | ATOM | 3762 | H1 | H2O | 12 | 17.417 | 40.675 | 50.306 | 1.00 | 0.00 | W |
| | ATOM | 3763 | H2 | H2O | 12 | 18.696 | 39.974 | 50.712 | 1.00 | 0.00 | W |
| | ATOM | 3764 | OH2 | H2O | 13 | 21.562 | 51.184 | 21.243 | 1.00 | 25.48 | W |
| | ATOM | 3765 | H1 | H2O | 13 | 21.072 | 51.974 | 21.467 | 1.00 | 0.00 | W |
| | ATOM | 3766 | H2 | H2O | 13 | 21.182 | 50.500 | 21.792 | 1.00 | 0.00 | W |
| 40 | ATOM | 3767 | OH2 | H2O | 14 | 7.521 | 51.792 | 47.594 | 1.00 | 15.43 | W |
| | ATOM | 3768 | H1 | H2O | 14 | 7.094 | 51.205 | 46.975 | 1.00 | 0.00 | W |
| | ATOM | 3769 | H2 | H2O | 14 | 8.187 | 52.245 | 47.075 | 1.00 | 0.00 | W |
| | ATOM | 3770 | OH2 | H2O | 15 | 10.086 | 64.032 | 53.718 | 1.00 | 28.77 | W |
| | ATOM | 3771 | H1 | H2O | 15 | 9.359 | 63.736 | 53.165 | 1.00 | 0.00 | W |
| 45 | ATOM | 3772 | H2 | H2O | 15 | 10.701 | 63.300 | 53.713 | 1.00 | 0.00 | W |
| | ATOM | 3773 | OH2 | H2O | 16 | 35.315 | 54.724 | 34.014 | 1.00 | 42.64 | W |
| | ATOM | 3774 | H1 | H2O | 16 | 36.015 | 55.349 | 33.832 | 1.00 | 0.00 | W |
| | ATOM | 3775 | H2 | H2O | 16 | 35.680 | 54.137 | 34.676 | 1.00 | 0.00 | W |
| | ATOM | 3776 | OH2 | H2O | 17 | 6.402 | 69.762 | 21.688 | 1.00 | 32.95 | W |
| 50 | ATOM | 3777 | H1 | H2O | 17 | 6.183 | 70.430 | 22.334 | 1.00 | 0.00 | W |
| | ATOM | 3778 | H2 | H2O | 17 | 6.335 | 70.208 | 20.844 | 1.00 | 0.00 | W |
| | ATOM | 3779 | OH2 | H2O | 18 | 14.632 | 41.929 | 43.654 | 1.00 | 18.32 | W |
| | ATOM | 3780 | H1 | H2O | 18 | 15.167 | 42.282 | 44.368 | 1.00 | 0.00 | W |
| | ATOM | 3781 | H2 | H2O | 18 | 15.258 | 41.449 | 43.107 | 1.00 | 0.00 | W |
| 55 | ATOM | 3782 | OH2 | H2O | 19 | 40.329 | 91.816 | -7.396 | 1.00 | 25.37 | W |
| | ATOM | 3783 | H1 | H2O | 19 | 39.913 | 91.345 | -6.675 | 1.00 | 0.00 | W |
| | ATOM | 3784 | H2 | H2O | 19 | 40.631 | 92.636 | -7.004 | 1.00 | 0.00 | W |
| | ATOM | 3785 | OH2 | H2O | 20 | 6.640 | 73.014 | 46.415 | 1.00 | 33.60 | W |
| | ATOM | 3786 | H1 | H2O | 20 | 6.738 | 72.084 | 46.624 | 1.00 | 0.00 | W |
| 60 | ATOM | 3787 | H2 | H2O | 20 | 6.989 | 73.098 | 45.531 | 1.00 | 0.00 | W |
| | ATOM | 3788 | OH2 | H2O | 21 | 37.583 | 68.788 | 40.034 | 1.00 | 36.96 | W |
| | ATOM | 3789 | H1 | H2O | 21 | 37.026 | 69.000 | 39.287 | 1.00 | 0.00 | W |
| | ATOM | 3790 | H2 | H2O | 21 | 38.300 | 68.285 | 39.657 | 1.00 | 0.00 | W |
| | ATOM | 3791 | OH2 | H2O | 22 | 5.165 | 71.647 | 48.591 | 1.00 | 35.16 | W |
| 65 | ATOM | 3792 | H1 | H2O | 22 | 5.385 | 70.721 | 48.682 | 1.00 | 0.00 | W |
| | ATOM | 3793 | H2 | H2O | 22 | 4.625 | 71.844 | 49.355 | 1.00 | 0.00 | W |
| | ATOM | 3794 | OH2 | H2O | 23 | 22.348 | 84.835 | 16.567 | 1.00 | 16.19 | W |
| | ATOM | 3795 | H1 | H2O | 23 | 23.280 | 84.637 | 16.464 | 1.00 | 0.00 | W |
| | ATOM | 3796 | H2 | H2O | 23 | 22.114 | 85.295 | 15.758 | 1.00 | 0.00 | W |
| 70 | ATOM | 3797 | OH2 | H2O | 24 | 15.889 | 49.740 | 39.303 | 1.00 | 19.38 | W |
| | ATOM | 3798 | H1 | H2O | 24 | 16.319 | 48.932 | 39.026 | 1.00 | 0.00 | W |
| | ATOM | 3799 | H2 | H2O | 24 | 15.010 | 49.471 | 39.561 | 1.00 | 0.00 | W |
| | ATOM | 3800 | OH2 | H2O | 25 | 37.655 | 61.332 | 27.513 | 1.00 | 31.70 | W |
| | ATOM | 3801 | H1 | H2O | 25 | 36.886 | 61.727 | 27.931 | 1.00 | 0.00 | W |
| 70 | ATOM | 3802 | H2 | H2O | 25 | 37.861 | 60.575 | 28.057 | 1.00 | 0.00 | W |
| | ATOM | 3803 | OH2 | H2O | 26 | 17.980 | 71.537 | 17.982 | 1.00 | 39.05 | W |
| | ATOM | 3804 | H1 | H2O | 26 | 17.960 | 70.901 | 17.268 | 1.00 | 0.00 | W |

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|----|------|------|-----|-----|----|--------|--------|---------|------|-------|---|
| 5 | ATOM | 3805 | H2 | H2O | 26 | 18.160 | 71.014 | 18.764 | 1.00 | 0.00 | W |
| | ATOM | 3806 | OH2 | H2O | 27 | 12.412 | 74.571 | -14.438 | 1.00 | 54.13 | W |
| | ATOM | 3807 | H1 | H2O | 27 | 11.645 | 74.040 | -14.647 | 1.00 | 0.00 | W |
| | ATOM | 3808 | H2 | H2O | 27 | 12.947 | 74.009 | -13.875 | 1.00 | 0.00 | W |
| | ATOM | 3809 | OH2 | H2O | 28 | 35.093 | 93.688 | 9.513 | 1.00 | 49.07 | W |
| 10 | ATOM | 3810 | H1 | H2O | 28 | 34.158 | 93.901 | 9.502 | 1.00 | 0.00 | W |
| | ATOM | 3811 | H2 | H2O | 28 | 35.143 | 92.843 | 9.955 | 1.00 | 0.00 | W |
| | ATOM | 3812 | OH2 | H2O | 29 | 27.557 | 67.319 | 47.587 | 1.00 | 20.63 | W |
| | ATOM | 3813 | H1 | H2O | 29 | 28.387 | 67.684 | 47.271 | 1.00 | 0.00 | W |
| | ATOM | 3814 | H2 | H2O | 29 | 27.650 | 66.377 | 47.466 | 1.00 | 0.00 | W |
| 15 | ATOM | 3815 | OH2 | H2O | 30 | 12.145 | 50.693 | 37.668 | 1.00 | 22.09 | W |
| | ATOM | 3816 | H1 | H2O | 30 | 12.508 | 49.987 | 38.209 | 1.00 | 0.00 | W |
| | ATOM | 3817 | H2 | H2O | 30 | 12.370 | 51.493 | 38.131 | 1.00 | 0.00 | W |
| | ATOM | 3818 | OH2 | H2O | 31 | 29.496 | 59.286 | 42.408 | 1.00 | 37.05 | W |
| | ATOM | 3819 | H1 | H2O | 31 | 30.012 | 59.213 | 43.211 | 1.00 | 0.00 | W |
| 20 | ATOM | 3820 | H2 | H2O | 31 | 29.640 | 60.183 | 42.110 | 1.00 | 0.00 | W |
| | ATOM | 3821 | OH2 | H2O | 32 | 28.197 | 52.345 | 43.775 | 1.00 | 24.75 | W |
| | ATOM | 3822 | H1 | H2O | 32 | 28.094 | 52.722 | 42.902 | 1.00 | 0.00 | W |
| | ATOM | 3823 | H2 | H2O | 32 | 28.541 | 51.469 | 43.622 | 1.00 | 0.00 | W |
| | ATOM | 3824 | OH2 | H2O | 33 | 23.054 | 77.785 | -19.613 | 1.00 | 54.17 | W |
| 25 | ATOM | 3825 | H1 | H2O | 33 | 23.018 | 77.086 | -20.264 | 1.00 | 0.00 | W |
| | ATOM | 3826 | H2 | H2O | 33 | 23.144 | 78.588 | -20.124 | 1.00 | 0.00 | W |
| | ATOM | 3827 | OH2 | H2O | 34 | 11.508 | 89.358 | -0.033 | 1.00 | 89.65 | W |
| | ATOM | 3828 | H1 | H2O | 34 | 10.947 | 90.015 | 0.378 | 1.00 | 0.00 | W |
| | ATOM | 3829 | H2 | H2O | 34 | 11.860 | 88.850 | 0.697 | 1.00 | 0.00 | W |
| 30 | ATOM | 3830 | OH2 | H2O | 35 | 11.641 | 45.393 | 37.448 | 1.00 | 51.14 | W |
| | ATOM | 3831 | H1 | H2O | 35 | 11.020 | 45.208 | 36.743 | 1.00 | 0.00 | W |
| | ATOM | 3832 | H2 | H2O | 35 | 11.965 | 44.531 | 37.713 | 1.00 | 0.00 | W |
| | ATOM | 3833 | OH2 | H2O | 36 | 20.569 | 40.000 | 37.790 | 1.00 | 29.17 | W |
| | ATOM | 3834 | H1 | H2O | 36 | 20.797 | 40.503 | 37.007 | 1.00 | 0.00 | W |
| 35 | ATOM | 3835 | H2 | H2O | 36 | 20.901 | 40.523 | 38.517 | 1.00 | 0.00 | W |
| | ATOM | 3836 | OH2 | H2O | 37 | 24.685 | 71.120 | -9.820 | 1.00 | 43.88 | W |
| | ATOM | 3837 | H1 | H2O | 37 | 25.328 | 70.841 | -9.165 | 1.00 | 0.00 | W |
| | ATOM | 3838 | H2 | H2O | 37 | 24.632 | 70.379 | -10.426 | 1.00 | 0.00 | W |
| | ATOM | 3839 | OH2 | H2O | 38 | 17.308 | 85.319 | 37.723 | 1.00 | 34.44 | W |
| 40 | ATOM | 3840 | H1 | H2O | 38 | 18.044 | 85.879 | 37.954 | 1.00 | 0.00 | W |
| | ATOM | 3841 | H2 | H2O | 38 | 17.596 | 84.434 | 37.953 | 1.00 | 0.00 | W |
| | ATOM | 3842 | OH2 | H2O | 39 | 12.687 | 42.769 | 41.100 | 1.00 | 28.15 | W |
| | ATOM | 3843 | H1 | H2O | 39 | 12.510 | 41.844 | 40.940 | 1.00 | 0.00 | W |
| | ATOM | 3844 | H2 | H2O | 39 | 11.922 | 43.225 | 40.743 | 1.00 | 0.00 | W |
| 45 | ATOM | 3845 | OH2 | H2O | 40 | 17.331 | 86.756 | 34.308 | 1.00 | 14.85 | W |
| | ATOM | 3846 | H1 | H2O | 40 | 18.021 | 87.306 | 34.677 | 1.00 | 0.00 | W |
| | ATOM | 3847 | H2 | H2O | 40 | 17.772 | 85.936 | 34.083 | 1.00 | 0.00 | W |
| | ATOM | 3848 | OH2 | H2O | 41 | 11.389 | 77.413 | 34.219 | 1.00 | 13.24 | W |
| | ATOM | 3849 | H1 | H2O | 41 | 11.834 | 76.632 | 33.886 | 1.00 | 0.00 | W |
| 50 | ATOM | 3850 | H2 | H2O | 41 | 11.955 | 77.724 | 34.927 | 1.00 | 0.00 | W |
| | ATOM | 3851 | OH2 | H2O | 42 | 22.064 | 47.418 | 49.189 | 1.00 | 21.90 | W |
| | ATOM | 3852 | H1 | H2O | 42 | 22.578 | 47.067 | 49.916 | 1.00 | 0.00 | W |
| | ATOM | 3853 | H2 | H2O | 42 | 21.955 | 48.346 | 49.399 | 1.00 | 0.00 | W |
| | ATOM | 3854 | OH2 | H2O | 43 | 42.304 | 89.935 | -4.829 | 1.00 | 41.26 | W |
| 55 | ATOM | 3855 | H1 | H2O | 43 | 42.968 | 90.334 | -4.263 | 1.00 | 0.00 | W |
| | ATOM | 3856 | H2 | H2O | 43 | 41.497 | 90.399 | -4.614 | 1.00 | 0.00 | W |
| | ATOM | 3857 | OH2 | H2O | 44 | 20.332 | 50.701 | 49.638 | 1.00 | 34.52 | W |
| | ATOM | 3858 | H1 | H2O | 44 | 20.304 | 50.701 | 48.682 | 1.00 | 0.00 | W |
| | ATOM | 3859 | H2 | H2O | 44 | 20.709 | 51.553 | 49.866 | 1.00 | 0.00 | W |
| 60 | ATOM | 3860 | OH2 | H2O | 45 | 29.753 | 79.163 | 20.128 | 1.00 | 29.41 | W |
| | ATOM | 3861 | H1 | H2O | 45 | 29.861 | 79.995 | 20.588 | 1.00 | 0.00 | W |
| | ATOM | 3862 | H2 | H2O | 45 | 30.517 | 78.646 | 20.388 | 1.00 | 0.00 | W |
| | ATOM | 3863 | OH2 | H2O | 46 | 21.428 | 84.063 | 13.081 | 1.00 | 37.53 | W |
| | ATOM | 3864 | H1 | H2O | 46 | 21.980 | 83.848 | 12.332 | 1.00 | 0.00 | W |
| 65 | ATOM | 3865 | H2 | H2O | 46 | 22.024 | 84.033 | 13.833 | 1.00 | 0.00 | W |
| | ATOM | 3866 | OH2 | H2O | 47 | 44.014 | 87.180 | 0.493 | 1.00 | 42.34 | W |
| | ATOM | 3867 | H1 | H2O | 47 | 44.816 | 87.537 | 0.112 | 1.00 | 0.00 | W |
| | ATOM | 3868 | H2 | H2O | 47 | 44.255 | 86.949 | 1.390 | 1.00 | 0.00 | W |
| | ATOM | 3869 | OH2 | H2O | 48 | 10.349 | 58.686 | 20.367 | 1.00 | 54.51 | W |
| 70 | ATOM | 3870 | H1 | H2O | 48 | 11.088 | 58.206 | 20.745 | 1.00 | 0.00 | W |
| | ATOM | 3871 | H2 | H2O | 48 | 10.744 | 59.467 | 19.982 | 1.00 | 0.00 | W |
| | ATOM | 3872 | OH2 | H2O | 50 | 23.990 | 56.220 | 51.509 | 1.00 | 25.41 | W |
| | ATOM | 3873 | H1 | H2O | 50 | 23.268 | 55.601 | 51.628 | 1.00 | 0.00 | W |
| | ATOM | 3874 | H2 | H2O | 50 | 24.178 | 56.195 | 50.573 | 1.00 | 0.00 | W |
| | ATOM | 3875 | OH2 | H2O | 51 | 14.872 | 75.264 | -7.889 | 1.00 | 34.60 | W |
| | ATOM | 3876 | H1 | H2O | 51 | 15.737 | 75.461 | -8.249 | 1.00 | 0.00 | W |
| | ATOM | 3877 | H2 | H2O | 51 | 15.004 | 75.262 | -6.940 | 1.00 | 0.00 | W |

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|----|------|------|-----|-----|----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 3878 | OH2 | H2O | 52 | 29.495 | 53.936 | 48.249 | 1.00 | 35.09 | W |
| | ATOM | 3879 | H1 | H2O | 52 | 30.382 | 53.691 | 48.511 | 1.00 | 0.00 | W |
| | ATOM | 3880 | H2 | H2O | 52 | 28.980 | 53.881 | 49.050 | 1.00 | 0.00 | W |
| | ATOM | 3881 | OH2 | H2O | 53 | 23.913 | 39.862 | 34.279 | 1.00 | 24.69 | W |
| | ATOM | 3882 | H1 | H2O | 53 | 23.928 | 40.573 | 34.917 | 1.00 | 0.00 | W |
| | ATOM | 3883 | H2 | H2O | 53 | 22.981 | 39.718 | 34.101 | 1.00 | 0.00 | W |
| | ATOM | 3884 | OH2 | H2O | 54 | 27.855 | 38.735 | 36.184 | 1.00 | 41.97 | W |
| 10 | ATOM | 3885 | H1 | H2O | 54 | 27.501 | 37.874 | 35.965 | 1.00 | 0.00 | W |
| | ATOM | 3886 | H2 | H2O | 54 | 27.094 | 39.319 | 36.159 | 1.00 | 0.00 | W |
| | ATOM | 3887 | OH2 | H2O | 55 | 14.443 | 71.878 | 19.001 | 1.00 | 43.17 | W |
| | ATOM | 3888 | H1 | H2O | 55 | 13.698 | 71.493 | 18.533 | 1.00 | 0.00 | W |
| | ATOM | 3889 | H2 | H2O | 55 | 14.053 | 72.271 | 19.782 | 1.00 | 0.00 | W |
| | ATOM | 3890 | OH2 | H2O | 56 | 9.281 | 50.087 | 37.191 | 1.00 | 22.03 | W |
| | ATOM | 3891 | H1 | H2O | 56 | 10.124 | 49.922 | 36.769 | 1.00 | 0.00 | W |
| 15 | ATOM | 3892 | H2 | H2O | 56 | 9.351 | 49.660 | 38.045 | 1.00 | 0.00 | W |
| | ATOM | 3893 | OH2 | H2O | 57 | 22.892 | 77.131 | 20.524 | 1.00 | 38.72 | W |
| | ATOM | 3894 | H1 | H2O | 57 | 22.303 | 76.460 | 20.869 | 1.00 | 0.00 | W |
| | ATOM | 3895 | H2 | H2O | 57 | 22.962 | 76.933 | 19.591 | 1.00 | 0.00 | W |
| | ATOM | 3896 | OH2 | H2O | 58 | 38.306 | 78.270 | 13.963 | 1.00 | 28.31 | W |
| | ATOM | 3897 | H1 | H2O | 58 | 38.886 | 77.518 | 14.102 | 1.00 | 0.00 | W |
| | ATOM | 3898 | H2 | H2O | 58 | 37.541 | 77.899 | 13.520 | 1.00 | 0.00 | W |
| 20 | ATOM | 3899 | OH2 | H2O | 59 | 10.937 | 66.046 | 49.581 | 1.00 | 34.62 | W |
| | ATOM | 3900 | H1 | H2O | 59 | 11.082 | 66.814 | 49.032 | 1.00 | 0.00 | W |
| | ATOM | 3901 | H2 | H2O | 59 | 11.613 | 65.426 | 49.320 | 1.00 | 0.00 | W |
| | ATOM | 3902 | OH2 | H2O | 60 | 40.917 | 80.629 | -4.294 | 1.00 | 39.29 | W |
| | ATOM | 3903 | H1 | H2O | 60 | 40.941 | 81.265 | -5.010 | 1.00 | 0.00 | W |
| | ATOM | 3904 | H2 | H2O | 60 | 41.832 | 80.403 | -4.141 | 1.00 | 0.00 | W |
| | ATOM | 3905 | OH2 | H2O | 61 | 37.462 | 76.032 | 26.379 | 1.00 | 35.75 | W |
| 30 | ATOM | 3906 | H1 | H2O | 61 | 37.318 | 75.396 | 27.075 | 1.00 | 0.00 | W |
| | ATOM | 3907 | H2 | H2O | 61 | 36.637 | 76.059 | 25.897 | 1.00 | 0.00 | W |
| | ATOM | 3908 | OH2 | H2O | 62 | 12.194 | 92.917 | 7.443 | 1.00 | 26.35 | W |
| | ATOM | 3909 | H1 | H2O | 62 | 12.299 | 93.860 | 7.569 | 1.00 | 0.00 | W |
| | ATOM | 3910 | H2 | H2O | 62 | 12.553 | 92.749 | 6.576 | 1.00 | 0.00 | W |
| | ATOM | 3911 | OH2 | H2O | 63 | 10.746 | 48.472 | 38.472 | 1.00 | 32.24 | W |
| | ATOM | 3912 | H1 | H2O | 63 | 11.037 | 49.361 | 38.660 | 1.00 | 0.00 | W |
| 35 | ATOM | 3913 | H2 | H2O | 63 | 11.406 | 47.907 | 38.868 | 1.00 | 0.00 | W |
| | ATOM | 3914 | OH2 | H2O | 64 | 24.609 | 73.773 | 41.569 | 1.00 | 29.16 | W |
| | ATOM | 3915 | H1 | H2O | 64 | 24.846 | 74.155 | 42.417 | 1.00 | 0.00 | W |
| | ATOM | 3916 | H2 | H2O | 64 | 25.433 | 73.754 | 41.081 | 1.00 | 0.00 | W |
| | ATOM | 3917 | OH2 | H2O | 65 | 30.012 | 66.185 | -8.084 | 1.00 | 59.17 | W |
| | ATOM | 3918 | H1 | H2O | 65 | 30.800 | 66.596 | -7.731 | 1.00 | 0.00 | W |
| | ATOM | 3919 | H2 | H2O | 65 | 29.658 | 66.832 | -6.697 | 1.00 | 0.00 | W |
| 45 | ATOM | 3920 | OH2 | H2O | 66 | 31.620 | 57.288 | 44.605 | 1.00 | 33.39 | W |
| | ATOM | 3921 | H1 | H2O | 66 | 30.791 | 56.867 | 44.837 | 1.00 | 0.00 | W |
| | ATOM | 3922 | H2 | H2O | 66 | 31.532 | 57.494 | 43.676 | 1.00 | 0.00 | W |
| | ATOM | 3923 | OH2 | H2O | 67 | 18.628 | 82.133 | 47.615 | 1.00 | 41.34 | W |
| | ATOM | 3924 | H1 | H2O | 67 | 19.144 | 81.345 | 47.779 | 1.00 | 0.00 | W |
| | ATOM | 3925 | H2 | H2O | 67 | 18.596 | 82.582 | 48.458 | 1.00 | 0.00 | W |
| | ATOM | 3926 | OH2 | H2O | 68 | 26.118 | 86.559 | 16.428 | 1.00 | 16.27 | W |
| 50 | ATOM | 3927 | H1 | H2O | 68 | 25.731 | 86.540 | 17.305 | 1.00 | 0.00 | W |
| | ATOM | 3928 | H2 | H2O | 68 | 26.764 | 87.261 | 16.467 | 1.00 | 0.00 | W |
| | ATOM | 3929 | OH2 | H2O | 69 | 6.149 | 45.998 | 26.772 | 1.00 | 58.89 | W |
| | ATOM | 3930 | H1 | H2O | 69 | 6.523 | 46.223 | 27.625 | 1.00 | 0.00 | W |
| | ATOM | 3931 | H2 | H2O | 69 | 5.200 | 46.037 | 26.914 | 1.00 | 0.00 | W |
| | ATOM | 3932 | OH2 | H2O | 70 | 7.387 | 86.734 | 36.372 | 1.00 | 26.69 | W |
| | ATOM | 3933 | H1 | H2O | 70 | 7.690 | 87.232 | 35.613 | 1.00 | 0.00 | W |
| 60 | ATOM | 3934 | H2 | H2O | 70 | 6.557 | 87.153 | 36.615 | 1.00 | 0.00 | W |
| | ATOM | 3935 | OH2 | H2O | 71 | 19.016 | 50.608 | 41.020 | 1.00 | 20.12 | W |
| | ATOM | 3936 | H1 | H2O | 71 | 19.744 | 51.094 | 41.405 | 1.00 | 0.00 | W |
| | ATOM | 3937 | H2 | H2O | 71 | 18.765 | 51.119 | 40.254 | 1.00 | 0.00 | W |
| | ATOM | 3938 | OH2 | H2O | 72 | 22.966 | 54.069 | 53.338 | 1.00 | 58.44 | W |
| | ATOM | 3939 | H1 | H2O | 72 | 22.736 | 53.762 | 54.218 | 1.00 | 0.00 | W |
| | ATOM | 3940 | H2 | H2O | 72 | 23.801 | 54.525 | 53.458 | 1.00 | 0.00 | W |
| 65 | ATOM | 3941 | OH2 | H2O | 73 | 32.935 | 84.107 | 34.520 | 1.00 | 38.39 | W |
| | ATOM | 3942 | H1 | H2O | 73 | 32.932 | 85.062 | 34.520 | 1.00 | 0.00 | W |
| | ATOM | 3943 | H2 | H2O | 73 | 32.932 | 83.865 | 33.593 | 1.00 | 0.00 | W |
| | ATOM | 3944 | OH2 | H2O | 74 | 15.144 | 50.152 | 34.763 | 1.00 | 15.36 | W |
| | ATOM | 3945 | H1 | H2O | 74 | 15.994 | 49.728 | 34.642 | 1.00 | 0.00 | W |
| | ATOM | 3946 | H2 | H2O | 74 | 14.963 | 50.062 | 35.700 | 1.00 | 0.00 | W |
| | ATOM | 3947 | OH2 | H2O | 75 | 39.834 | 73.517 | 37.279 | 1.00 | 21.08 | W |
| 70 | ATOM | 3948 | H1 | H2O | 75 | 39.093 | 73.212 | 37.805 | 1.00 | 0.00 | W |
| | ATOM | 3949 | H2 | H2O | 75 | 39.719 | 74.465 | 37.239 | 1.00 | 0.00 | W |
| | ATOM | 3950 | OH2 | H2O | 76 | 5.621 | 49.847 | 47.235 | 1.00 | 36.63 | W |

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|----|------|------|-----|-----|-----|--------|--------|---------|------|-------|---|
| | ATOM | 3951 | H1 | H2O | 76 | 5.682 | 50.181 | 48.127 | 1.00 | 0.00 | W |
| | ATOM | 3952 | H2 | H2O | 76 | 6.291 | 50.328 | 46.749 | 1.00 | 0.00 | W |
| | ATOM | 3953 | OH2 | H2O | 77 | 20.855 | 42.150 | 47.963 | 1.00 | 45.89 | W |
| 5 | ATOM | 3954 | H1 | H2O | 77 | 21.782 | 42.249 | 47.739 | 1.00 | 0.00 | W |
| | ATOM | 3955 | H2 | H2O | 77 | 20.797 | 41.284 | 48.366 | 1.00 | 0.00 | W |
| | ATOM | 3956 | OH2 | H2O | 78 | 8.330 | 65.636 | 18.869 | 1.00 | 38.49 | W |
| | ATOM | 3957 | H1 | H2O | 78 | 8.581 | 66.186 | 18.125 | 1.00 | 0.00 | W |
| | ATOM | 3958 | H2 | H2O | 78 | 8.184 | 66.254 | 19.584 | 1.00 | 0.00 | W |
| 10 | ATOM | 3959 | OH2 | H2O | 79 | 37.225 | 73.080 | 47.421 | 1.00 | 42.94 | W |
| | ATOM | 3960 | H1 | H2O | 79 | 37.775 | 72.667 | 46.755 | 1.00 | 0.00 | W |
| | ATOM | 3961 | H2 | H2O | 79 | 36.353 | 73.108 | 47.030 | 1.00 | 0.00 | W |
| | ATOM | 3962 | OH2 | H2O | 80 | 36.019 | 65.979 | 41.953 | 1.00 | 34.15 | W |
| | ATOM | 3963 | H1 | H2O | 80 | 36.913 | 65.996 | 42.303 | 1.00 | 0.00 | W |
| 15 | ATOM | 3964 | H2 | H2O | 80 | 35.821 | 65.048 | 41.856 | 1.00 | 0.00 | W |
| | ATOM | 3965 | OH2 | H2O | 81 | 37.936 | 72.735 | -2.902 | 1.00 | 58.65 | W |
| | ATOM | 3966 | H1 | H2O | 81 | 38.631 | 73.117 | -2.367 | 1.00 | 0.00 | W |
| | ATOM | 3967 | H2 | H2O | 81 | 37.913 | 73.277 | -3.690 | 1.00 | 0.00 | W |
| | ATOM | 3968 | OH2 | H2O | 82 | 23.143 | 50.854 | 55.229 | 1.00 | 73.08 | W |
| 20 | ATOM | 3969 | H1 | H2O | 82 | 22.200 | 50.699 | 55.185 | 1.00 | 0.00 | W |
| | ATOM | 3970 | H2 | H2O | 82 | 23.429 | 50.377 | 56.008 | 1.00 | 0.00 | W |
| | ATOM | 3971 | OH2 | H2O | 83 | 35.270 | 96.894 | -8.992 | 1.00 | 46.37 | W |
| | ATOM | 3972 | H1 | H2O | 83 | 34.385 | 97.082 | -9.298 | 1.00 | 0.00 | W |
| | ATOM | 3973 | H2 | H2O | 83 | 35.800 | 97.621 | -9.320 | 1.00 | 0.00 | W |
| 25 | ATOM | 3974 | OH2 | H2O | 84 | 34.683 | 68.046 | 40.254 | 1.00 | 41.87 | W |
| | ATOM | 3975 | H1 | H2O | 84 | 35.001 | 67.185 | 39.981 | 1.00 | 0.00 | W |
| | ATOM | 3976 | H2 | H2O | 84 | 33.743 | 68.022 | 40.069 | 1.00 | 0.00 | W |
| | ATOM | 3977 | OH2 | H2O | 85 | 7.937 | 93.884 | 8.479 | 1.00 | 67.26 | W |
| | ATOM | 3978 | H1 | H2O | 85 | 8.505 | 93.128 | 8.331 | 1.00 | 0.00 | W |
| 30 | ATOM | 3979 | H2 | H2O | 85 | 7.793 | 94.250 | 7.607 | 1.00 | 0.00 | W |
| | ATOM | 3980 | OH2 | H2O | 86 | 41.437 | 88.270 | 5.694 | 1.00 | 43.07 | W |
| | ATOM | 3981 | H1 | H2O | 86 | 40.650 | 88.680 | 6.057 | 1.00 | 0.00 | W |
| | ATOM | 3982 | H2 | H2O | 86 | 41.183 | 87.355 | 5.556 | 1.00 | 0.00 | W |
| | ATOM | 3983 | OH2 | H2O | 87 | 18.418 | 89.968 | 41.295 | 1.00 | 50.98 | W |
| 35 | ATOM | 3984 | H1 | H2O | 87 | 19.346 | 89.974 | 41.525 | 1.00 | 0.00 | W |
| | ATOM | 3985 | H2 | H2O | 87 | 18.287 | 89.127 | 40.854 | 1.00 | 0.00 | W |
| | ATOM | 3986 | OH2 | H2O | 88 | 15.346 | 97.033 | 5.772 | 1.00 | 51.64 | W |
| | ATOM | 3987 | H1 | H2O | 88 | 14.535 | 97.052 | 5.262 | 1.00 | 0.00 | W |
| | ATOM | 3988 | H2 | H2O | 88 | 15.780 | 96.224 | 5.502 | 1.00 | 0.00 | W |
| 40 | ATOM | 3989 | OH2 | H2O | 89 | 47.753 | 89.370 | -3.781 | 1.00 | 37.41 | W |
| | ATOM | 3990 | H1 | H2O | 89 | 47.756 | 90.330 | -3.781 | 1.00 | 0.00 | W |
| | ATOM | 3991 | H2 | H2O | 89 | 47.756 | 89.133 | -4.708 | 1.00 | 0.00 | W |
| | ATOM | 3992 | OH2 | H2O | 90 | 17.822 | 70.217 | 21.038 | 1.00 | 53.57 | W |
| | ATOM | 3993 | H1 | H2O | 90 | 18.493 | 70.890 | 21.166 | 1.00 | 0.00 | W |
| 45 | ATOM | 3994 | H2 | H2O | 90 | 17.151 | 70.426 | 21.692 | 1.00 | 0.00 | W |
| | ATOM | 3995 | OH2 | H2O | 91 | 2.696 | 51.590 | 41.944 | 1.00 | 46.78 | W |
| | ATOM | 3996 | H1 | H2O | 91 | 1.893 | 51.743 | 42.439 | 1.00 | 0.00 | W |
| | ATOM | 3997 | H2 | H2O | 91 | 3.400 | 51.837 | 42.544 | 1.00 | 0.00 | W |
| | ATOM | 3998 | OH2 | H2O | 95 | 34.676 | 75.860 | 41.073 | 1.00 | 39.50 | W |
| 50 | ATOM | 3999 | H1 | H2O | 95 | 35.228 | 75.793 | 40.290 | 1.00 | 0.00 | W |
| | ATOM | 4000 | H2 | H2O | 95 | 34.453 | 74.957 | 41.286 | 1.00 | 0.00 | W |
| | ATOM | 4001 | OH2 | H2O | 96 | 39.675 | 76.625 | -9.371 | 1.00 | 56.41 | W |
| | ATOM | 4002 | H1 | H2O | 96 | 38.896 | 76.095 | -9.211 | 1.00 | 0.00 | W |
| | ATOM | 4003 | H2 | H2O | 96 | 40.385 | 75.984 | -9.456 | 1.00 | 0.00 | W |
| 55 | ATOM | 4004 | OH2 | H2O | 97 | 18.254 | 64.042 | 7.803 | 1.00 | 55.42 | W |
| | ATOM | 4005 | H1 | H2O | 97 | 18.067 | 64.981 | 7.768 | 1.00 | 0.00 | W |
| | ATOM | 4006 | H2 | H2O | 97 | 17.406 | 63.636 | 7.982 | 1.00 | 0.00 | W |
| | ATOM | 4007 | OH2 | H2O | 99 | 36.040 | 76.842 | 46.828 | 1.00 | 41.76 | W |
| | ATOM | 4008 | H1 | H2O | 99 | 35.612 | 76.180 | 46.290 | 1.00 | 0.00 | W |
| 60 | ATOM | 4009 | H2 | H2O | 99 | 35.367 | 77.514 | 46.962 | 1.00 | 0.00 | W |
| | ATOM | 4010 | OH2 | H2O | 100 | 39.087 | 90.744 | -12.653 | 1.00 | 50.93 | W |
| | ATOM | 4011 | H1 | H2O | 100 | 39.148 | 91.213 | -13.482 | 1.00 | 0.00 | W |
| | ATOM | 4012 | H2 | H2O | 100 | 39.394 | 91.370 | -11.997 | 1.00 | 0.00 | W |
| | ATOM | 4013 | OH2 | H2O | 102 | 34.315 | 73.486 | 18.013 | 1.00 | 32.56 | W |
| 65 | ATOM | 4014 | H1 | H2O | 102 | 34.941 | 73.597 | 17.299 | 1.00 | 0.00 | W |
| | ATOM | 4015 | H2 | H2O | 102 | 33.483 | 73.303 | 17.577 | 1.00 | 0.00 | W |
| | ATOM | 4016 | OH2 | H2O | 103 | 27.629 | 65.918 | 7.501 | 1.00 | 26.86 | W |
| | ATOM | 4017 | H1 | H2O | 103 | 26.981 | 65.607 | 8.130 | 1.00 | 0.00 | W |
| | ATOM | 4018 | H2 | H2O | 103 | 28.387 | 65.342 | 7.634 | 1.00 | 0.00 | W |
| 70 | ATOM | 4019 | OH2 | H2O | 104 | 30.549 | 69.755 | -10.939 | 1.00 | 52.39 | W |
| | ATOM | 4020 | H1 | H2O | 104 | 30.082 | 70.440 | -11.415 | 1.00 | 0.00 | W |
| | ATOM | 4021 | H2 | H2O | 104 | 30.530 | 68.998 | -11.524 | 1.00 | 0.00 | W |
| | ATOM | 4022 | OH2 | H2O | 105 | 34.538 | 71.979 | 38.560 | 1.00 | 30.69 | W |
| | ATOM | 4023 | H1 | H2O | 105 | 33.720 | 72.302 | 38.185 | 1.00 | 0.00 | W |

| | | | | | | | | | | | |
|----|------|------|-----|-----|-----|--------|---------|---------|------|-------|---|
| 5 | ATOM | 4024 | H2 | H2O | 105 | 34.317 | 71.734 | 39.455 | 1.00 | 0.00 | W |
| | ATOM | 4025 | OH2 | H2O | 106 | 31.168 | 67.923 | 13.585 | 1.00 | 47.02 | W |
| | ATOM | 4026 | H1 | H2O | 106 | 31.193 | 67.876 | 14.540 | 1.00 | 0.00 | W |
| | ATOM | 4027 | H2 | H2O | 106 | 30.514 | 68.599 | 13.396 | 1.00 | 0.00 | W |
| | ATOM | 4028 | OH2 | H2O | 107 | 32.794 | 63.732 | 44.548 | 1.00 | 33.54 | W |
| 10 | ATOM | 4029 | H1 | H2O | 107 | 32.546 | 63.550 | 45.458 | 1.00 | 0.00 | W |
| | ATOM | 4030 | H2 | H2O | 107 | 33.687 | 63.411 | 44.472 | 1.00 | 0.00 | W |
| | ATOM | 4031 | OH2 | H2O | 108 | 19.475 | 88.576 | 35.346 | 1.00 | 35.25 | W |
| | ATOM | 4032 | H1 | H2O | 108 | 19.617 | 88.129 | 34.508 | 1.00 | 0.00 | W |
| | ATOM | 4033 | H2 | H2O | 108 | 20.226 | 88.319 | 35.881 | 1.00 | 0.00 | W |
| 15 | ATOM | 4034 | OH2 | H2O | 109 | 23.864 | 52.354 | 23.080 | 1.00 | 48.58 | W |
| | ATOM | 4035 | H1 | H2O | 109 | 23.166 | 52.051 | 22.499 | 1.00 | 0.00 | W |
| | ATOM | 4036 | H2 | H2O | 109 | 23.422 | 52.922 | 23.711 | 1.00 | 0.00 | W |
| | ATOM | 4037 | OH2 | H2O | 110 | 31.956 | 52.640 | 32.308 | 1.00 | 51.66 | W |
| | ATOM | 4038 | H1 | H2O | 110 | 31.785 | 52.563 | 31.371 | 1.00 | 0.00 | W |
| 20 | ATOM | 4039 | H2 | H2O | 110 | 31.086 | 52.644 | 32.711 | 1.00 | 0.00 | W |
| | ATOM | 4040 | OH2 | H2O | 111 | 16.968 | 60.681 | 13.605 | 1.00 | 55.65 | W |
| | ATOM | 4041 | H1 | H2O | 111 | 16.618 | 60.785 | 12.718 | 1.00 | 0.00 | W |
| | ATOM | 4042 | H2 | H2O | 111 | 17.849 | 61.054 | 13.557 | 1.00 | 0.00 | W |
| | ATOM | 4043 | OH2 | H2O | 112 | 38.699 | 63.142 | 37.584 | 1.00 | 49.09 | W |
| 25 | ATOM | 4044 | H1 | H2O | 112 | 37.844 | 62.845 | 37.265 | 1.00 | 0.00 | W |
| | ATOM | 4045 | H2 | H2O | 112 | 39.233 | 62.347 | 37.604 | 1.00 | 0.00 | W |
| | ATOM | 4046 | OH2 | H2O | 113 | 31.344 | 57.427 | 39.398 | 1.00 | 37.73 | W |
| | ATOM | 4047 | H1 | H2O | 113 | 31.126 | 56.895 | 40.166 | 1.00 | 0.00 | W |
| | ATOM | 4048 | H2 | H2O | 113 | 30.552 | 57.933 | 39.226 | 1.00 | 0.00 | W |
| 30 | ATOM | 4049 | OH2 | H2O | 114 | 41.350 | 83.449 | -8.714 | 1.00 | 60.04 | W |
| | ATOM | 4050 | H1 | H2O | 114 | 41.043 | 83.752 | -9.569 | 1.00 | 0.00 | W |
| | ATOM | 4051 | H2 | H2O | 114 | 41.072 | 84.130 | -8.103 | 1.00 | 0.00 | W |
| | ATOM | 4052 | OH2 | H2O | 115 | 42.987 | 90.912 | 5.698 | 1.00 | 36.99 | W |
| | ATOM | 4053 | H1 | H2O | 115 | 42.742 | 89.993 | 5.572 | 1.00 | 0.00 | W |
| 35 | ATOM | 4054 | H2 | H2O | 115 | 43.930 | 90.888 | 5.853 | 1.00 | 0.00 | W |
| | ATOM | 4055 | OH2 | H2O | 118 | 27.240 | 71.465 | 53.783 | 1.00 | 33.44 | W |
| | ATOM | 4056 | H1 | H2O | 118 | 27.239 | 72.422 | 53.780 | 1.00 | 0.00 | W |
| | ATOM | 4057 | H2 | H2O | 118 | 27.239 | 71.225 | 52.853 | 1.00 | 0.00 | W |
| | ATOM | 4058 | OH2 | H2O | 119 | 11.225 | 50.304 | 22.316 | 1.00 | 55.33 | W |
| 40 | ATOM | 4059 | H1 | H2O | 119 | 11.185 | 51.196 | 22.657 | 1.00 | 0.00 | W |
| | ATOM | 4060 | H2 | H2O | 119 | 10.758 | 50.343 | 21.483 | 1.00 | 0.00 | W |
| | ATOM | 4061 | OH2 | H2O | 122 | 10.516 | 74.345 | 13.709 | 1.00 | 49.01 | W |
| | ATOM | 4062 | H1 | H2O | 122 | 11.305 | 74.880 | 13.770 | 1.00 | 0.00 | W |
| | ATOM | 4063 | H2 | H2O | 122 | 10.747 | 73.529 | 14.153 | 1.00 | 0.00 | W |
| 45 | ATOM | 4064 | OH2 | H2O | 123 | 21.221 | 81.929 | 43.450 | 1.00 | 35.78 | W |
| | ATOM | 4065 | H1 | H2O | 123 | 20.410 | 82.390 | 43.227 | 1.00 | 0.00 | W |
| | ATOM | 4066 | H2 | H2O | 123 | 21.623 | 82.469 | 44.129 | 1.00 | 0.00 | W |
| | ATOM | 4067 | OH2 | H2O | 125 | 26.901 | 87.147 | 37.889 | 1.00 | 67.29 | W |
| | ATOM | 4068 | H1 | H2O | 125 | 25.985 | 87.057 | 37.631 | 1.00 | 0.00 | W |
| 50 | ATOM | 4069 | H2 | H2O | 125 | 26.955 | 86.709 | 38.739 | 1.00 | 0.00 | W |
| | ATOM | 4070 | OH2 | H2O | 127 | 38.005 | 73.517 | 7.577 | 1.00 | 47.94 | W |
| | ATOM | 4071 | H1 | H2O | 127 | 38.835 | 73.559 | 7.101 | 1.00 | 0.00 | W |
| | ATOM | 4072 | H2 | H2O | 127 | 38.249 | 73.253 | 8.463 | 1.00 | 0.00 | W |
| | ATOM | 4073 | OH2 | H2O | 130 | 10.402 | 70.971 | 29.298 | 1.00 | 20.65 | W |
| 55 | ATOM | 4074 | H1 | H2O | 130 | 9.723 | 71.264 | 28.687 | 1.00 | 0.00 | W |
| | ATOM | 4075 | H2 | H2O | 130 | 10.159 | 71.385 | 30.132 | 1.00 | 0.00 | W |
| | ATOM | 4076 | OH2 | H2O | 132 | 5.650 | 81.404 | 36.223 | 1.00 | 27.14 | W |
| | ATOM | 4077 | H1 | H2O | 132 | 4.752 | 81.595 | 36.500 | 1.00 | 0.00 | W |
| | ATOM | 4078 | H2 | H2O | 132 | 6.195 | 81.776 | 36.918 | 1.00 | 0.00 | W |
| 60 | ATOM | 4079 | OH2 | H2O | 133 | 13.263 | 68.119 | 49.513 | 1.00 | 44.60 | W |
| | ATOM | 4080 | H1 | H2O | 133 | 13.357 | 67.240 | 49.144 | 1.00 | 0.00 | W |
| | ATOM | 4081 | H2 | H2O | 133 | 13.500 | 68.707 | 48.799 | 1.00 | 0.00 | W |
| | ATOM | 4082 | OH2 | H2O | 134 | 19.524 | 87.618 | -11.380 | 1.00 | 25.22 | W |
| | ATOM | 4083 | H1 | H2O | 134 | 19.588 | 86.908 | -10.742 | 1.00 | 0.00 | W |
| 65 | ATOM | 4084 | H2 | H2O | 134 | 18.725 | 87.424 | -11.875 | 1.00 | 0.00 | W |
| | ATOM | 4085 | OH2 | H2O | 135 | 40.212 | 59.845 | 25.750 | 1.00 | 51.43 | W |
| | ATOM | 4086 | H1 | H2O | 135 | 41.124 | 59.975 | 26.015 | 1.00 | 0.00 | W |
| | ATOM | 4087 | H2 | H2O | 135 | 40.235 | 59.869 | 24.793 | 1.00 | 0.00 | W |
| | ATOM | 4088 | OH2 | H2O | 136 | 19.922 | 100.636 | -9.493 | 1.00 | 47.67 | W |
| 70 | ATOM | 4089 | H1 | H2O | 136 | 19.113 | 101.141 | -9.422 | 1.00 | 0.00 | W |
| | ATOM | 4090 | H2 | H2O | 136 | 20.620 | 101.276 | -9.363 | 1.00 | 0.00 | W |
| | ATOM | 4091 | OH2 | H2O | 137 | 7.532 | 75.485 | 18.573 | 1.00 | 47.00 | W |
| | ATOM | 4092 | H1 | H2O | 137 | 7.714 | 76.396 | 18.784 | 1.00 | 0.00 | W |
| | ATOM | 4093 | H2 | H2O | 137 | 6.759 | 75.513 | 18.008 | 1.00 | 0.00 | W |
| 70 | ATOM | 4094 | OH2 | H2O | 139 | 25.465 | 59.184 | 52.290 | 1.00 | 28.76 | W |
| | ATOM | 4095 | H1 | H2O | 139 | 25.749 | 59.465 | 51.420 | 1.00 | 0.00 | W |
| | ATOM | 4096 | H2 | H2O | 139 | 24.512 | 59.318 | 52.281 | 1.00 | 0.00 | W |

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|----|------|------|-----|-----|-----|--------|---------|---------|------|-------|---|
| 5 | ATOM | 4097 | OH2 | H2O | 140 | 14.960 | 69.189 | 7.890 | 1.00 | 46.58 | W |
| | ATOM | 4098 | H1 | H2O | 140 | 14.139 | 69.668 | 7.972 | 1.00 | 0.00 | W |
| | ATOM | 4099 | H2 | H2O | 140 | 15.631 | 69.867 | 7.811 | 1.00 | 0.00 | W |
| | ATOM | 4100 | OH2 | H2O | 142 | 31.562 | 73.845 | 26.725 | 1.00 | 46.85 | W |
| | ATOM | 4101 | H1 | H2O | 142 | 30.757 | 74.357 | 26.741 | 1.00 | 0.00 | W |
| 10 | ATOM | 4102 | H2 | H2O | 142 | 31.916 | 73.978 | 25.843 | 1.00 | 0.00 | W |
| | ATOM | 4103 | OH2 | H2O | 143 | 24.525 | 81.714 | 35.572 | 1.00 | 45.84 | W |
| | ATOM | 4104 | H1 | H2O | 143 | 23.681 | 81.414 | 35.237 | 1.00 | 0.00 | W |
| | ATOM | 4105 | H2 | H2O | 143 | 25.142 | 81.535 | 34.862 | 1.00 | 0.00 | W |
| | ATOM | 4106 | OH2 | H2O | 144 | 30.404 | 37.547 | 38.155 | 1.00 | 49.49 | W |
| 15 | ATOM | 4107 | H1 | H2O | 144 | 31.040 | 37.919 | 38.772 | 1.00 | 0.00 | W |
| | ATOM | 4108 | H2 | H2O | 144 | 29.868 | 38.295 | 37.890 | 1.00 | 0.00 | W |
| | ATOM | 4109 | OH2 | H2O | 145 | 18.510 | 37.954 | 48.005 | 1.00 | 31.26 | W |
| | ATOM | 4110 | H1 | H2O | 145 | 18.573 | 37.366 | 48.753 | 1.00 | 0.00 | W |
| | ATOM | 4111 | H2 | H2O | 145 | 19.251 | 37.719 | 47.448 | 1.00 | 0.00 | W |
| 20 | ATOM | 4112 | OH2 | H2O | 148 | 21.454 | 103.453 | -11.072 | 1.00 | 69.13 | W |
| | ATOM | 4113 | H1 | H2O | 148 | 21.532 | 103.913 | -10.238 | 1.00 | 0.00 | W |
| | ATOM | 4114 | H2 | H2O | 148 | 20.530 | 103.207 | -11.127 | 1.00 | 0.00 | W |
| | ATOM | 4115 | OH2 | H2O | 149 | 30.616 | 69.892 | 11.062 | 1.00 | 59.13 | W |
| | ATOM | 4116 | H1 | H2O | 149 | 30.597 | 69.088 | 10.544 | 1.00 | 0.00 | W |
| 25 | ATOM | 4117 | H2 | H2O | 149 | 31.534 | 69.990 | 11.317 | 1.00 | 0.00 | W |
| | ATOM | 4118 | OH2 | H2O | 151 | 22.397 | 96.000 | -18.890 | 1.00 | 49.14 | W |
| | ATOM | 4119 | H1 | H2O | 151 | 22.660 | 96.162 | -19.796 | 1.00 | 0.00 | W |
| | ATOM | 4120 | H2 | H2O | 151 | 22.588 | 95.071 | -18.750 | 1.00 | 0.00 | W |
| | ATOM | 4121 | OH2 | H2O | 152 | 23.997 | 68.719 | -3.081 | 1.00 | 37.05 | W |
| 30 | ATOM | 4122 | H1 | H2O | 152 | 23.944 | 69.622 | -3.393 | 1.00 | 0.00 | W |
| | ATOM | 4123 | H2 | H2O | 152 | 23.498 | 68.717 | -2.264 | 1.00 | 0.00 | W |
| | ATOM | 4124 | OH2 | H2O | 153 | 6.761 | 78.049 | 41.002 | 1.00 | 44.92 | W |
| | ATOM | 4125 | H1 | H2O | 153 | 6.495 | 77.572 | 40.213 | 1.00 | 0.00 | W |
| | ATOM | 4126 | H2 | H2O | 153 | 7.695 | 77.879 | 41.080 | 1.00 | 0.00 | W |
| 35 | ATOM | 4127 | OH2 | H2O | 154 | 14.604 | 84.085 | 47.918 | 1.00 | 27.17 | W |
| | ATOM | 4128 | H1 | H2O | 154 | 14.800 | 83.921 | 48.839 | 1.00 | 0.00 | W |
| | ATOM | 4129 | H2 | H2O | 154 | 15.458 | 84.196 | 47.504 | 1.00 | 0.00 | W |
| | ATOM | 4130 | OH2 | H2O | 157 | 20.208 | 87.608 | 38.773 | 1.00 | 46.36 | W |
| | ATOM | 4131 | H1 | H2O | 157 | 19.447 | 88.077 | 38.424 | 1.00 | 0.00 | W |
| 40 | ATOM | 4132 | H2 | H2O | 157 | 20.838 | 88.299 | 38.980 | 1.00 | 0.00 | W |
| | ATOM | 4133 | OH2 | H2O | 161 | 27.786 | 81.756 | 30.433 | 1.00 | 20.04 | W |
| | ATOM | 4134 | H1 | H2O | 161 | 27.657 | 81.992 | 31.345 | 1.00 | 0.00 | W |
| | ATOM | 4135 | H2 | H2O | 161 | 27.013 | 81.230 | 30.207 | 1.00 | 0.00 | W |
| | ATOM | 4136 | OH2 | H2O | 162 | 25.545 | 41.107 | 41.204 | 1.00 | 39.67 | W |
| 45 | ATOM | 4137 | H1 | H2O | 162 | 26.123 | 40.371 | 41.410 | 1.00 | 0.00 | W |
| | ATOM | 4138 | H2 | H2O | 162 | 24.668 | 40.789 | 41.410 | 1.00 | 0.00 | W |
| | ATOM | 4139 | OH2 | H2O | 163 | 34.968 | 61.130 | 39.718 | 1.00 | 58.53 | W |
| | ATOM | 4140 | H1 | H2O | 163 | 35.625 | 61.220 | 40.410 | 1.00 | 0.00 | W |
| | ATOM | 4141 | H2 | H2O | 163 | 34.194 | 60.792 | 40.166 | 1.00 | 0.00 | W |
| 50 | ATOM | 4142 | OH2 | H2O | 164 | 31.867 | 61.174 | 40.931 | 1.00 | 30.31 | W |
| | ATOM | 4143 | H1 | H2O | 164 | 31.027 | 60.812 | 40.654 | 1.00 | 0.00 | W |
| | ATOM | 4144 | H2 | H2O | 164 | 31.803 | 61.239 | 41.882 | 1.00 | 0.00 | W |
| | ATOM | 4145 | OH2 | H2O | 165 | 18.529 | 51.777 | 47.785 | 1.00 | 26.36 | W |
| | ATOM | 4146 | H1 | H2O | 165 | 18.240 | 52.561 | 48.263 | 1.00 | 0.00 | W |
| 55 | ATOM | 4147 | H2 | H2O | 165 | 18.619 | 51.109 | 48.456 | 1.00 | 0.00 | W |
| | ATOM | 4148 | OH2 | H2O | 166 | 6.824 | 56.798 | 46.694 | 1.00 | 31.23 | W |
| | ATOM | 4149 | H1 | H2O | 166 | 7.339 | 56.878 | 47.493 | 1.00 | 0.00 | W |
| | ATOM | 4150 | H2 | H2O | 166 | 5.921 | 56.982 | 46.973 | 1.00 | 0.00 | W |
| | ATOM | 4151 | OH2 | H2O | 167 | 4.124 | 74.966 | 21.486 | 1.00 | 35.69 | W |
| 60 | ATOM | 4152 | H1 | H2O | 167 | 4.300 | 75.262 | 20.590 | 1.00 | 0.00 | W |
| | ATOM | 4153 | H2 | H2O | 167 | 4.736 | 75.467 | 22.026 | 1.00 | 0.00 | W |
| | ATOM | 4154 | OH2 | H2O | 168 | 23.115 | 81.286 | -19.644 | 1.00 | 56.66 | W |
| | ATOM | 4155 | H1 | H2O | 168 | 23.431 | 81.070 | -20.521 | 1.00 | 0.00 | W |
| | ATOM | 4156 | H2 | H2O | 168 | 23.194 | 80.469 | -19.152 | 1.00 | 0.00 | W |
| 65 | ATOM | 4157 | OH2 | H2O | 169 | 3.381 | 70.239 | 27.505 | 1.00 | 32.76 | W |
| | ATOM | 4158 | H1 | H2O | 169 | 2.709 | 70.126 | 26.830 | 1.00 | 0.00 | W |
| | ATOM | 4159 | H2 | H2O | 169 | 3.950 | 70.929 | 27.161 | 1.00 | 0.00 | W |
| | ATOM | 4160 | OH2 | H2O | 170 | 38.354 | 96.654 | -4.019 | 1.00 | 38.96 | W |
| | ATOM | 4161 | H1 | H2O | 170 | 38.897 | 97.181 | -4.602 | 1.00 | 0.00 | W |
| 70 | ATOM | 4162 | H2 | H2O | 170 | 38.910 | 95.925 | -3.757 | 1.00 | 0.00 | W |
| | ATOM | 4163 | OH2 | H2O | 171 | 31.765 | 75.253 | 24.200 | 1.00 | 35.79 | W |
| | ATOM | 4164 | H1 | H2O | 171 | 31.801 | 76.033 | 23.651 | 1.00 | 0.00 | W |
| | ATOM | 4165 | H2 | H2O | 171 | 32.622 | 74.840 | 24.093 | 1.00 | 0.00 | W |
| | ATOM | 4166 | OH2 | H2O | 172 | 30.112 | 51.159 | 46.701 | 1.00 | 42.99 | W |
| 70 | ATOM | 4167 | H1 | H2O | 172 | 29.550 | 51.828 | 47.094 | 1.00 | 0.00 | W |
| | ATOM | 4168 | H2 | H2O | 172 | 30.504 | 50.708 | 47.449 | 1.00 | 0.00 | W |
| | ATOM | 4169 | OH2 | H2O | 173 | 14.724 | 60.204 | 54.146 | 1.00 | 44.12 | W |

| | | | | | | | | | | | |
|----|------|------|-----|-----|-----|--------|--------|--------|------|-------|---|
| 5 | ATOM | 4170 | H1 | H2O | 173 | 13.852 | 60.500 | 54.408 | 1.00 | 0.00 | W |
| | ATOM | 4171 | H2 | H2O | 173 | 15.149 | 59.955 | 54.966 | 1.00 | 0.00 | W |
| | ATOM | 4172 | OH2 | H2O | 174 | 34.426 | 92.105 | 20.174 | 1.00 | 43.09 | W |
| | ATOM | 4173 | H1 | H2O | 174 | 33.995 | 92.193 | 19.323 | 1.00 | 0.00 | W |
| | ATOM | 4174 | H2 | H2O | 174 | 35.110 | 92.775 | 20.165 | 1.00 | 0.00 | W |
| 10 | ATOM | 4175 | OH2 | H2O | 175 | 15.079 | 77.472 | 19.106 | 1.00 | 26.05 | W |
| | ATOM | 4176 | H1 | H2O | 175 | 15.197 | 78.034 | 19.868 | 1.00 | 0.00 | W |
| | ATOM | 4177 | H2 | H2O | 175 | 14.807 | 76.627 | 19.465 | 1.00 | 0.00 | W |
| | ATOM | 4178 | OH2 | H2O | 176 | 4.428 | 65.813 | 39.483 | 1.00 | 41.04 | W |
| | ATOM | 4179 | H1 | H2O | 176 | 4.482 | 66.597 | 38.935 | 1.00 | 0.00 | W |
| 15 | ATOM | 4180 | H2 | H2O | 176 | 3.948 | 66.099 | 40.261 | 1.00 | 0.00 | W |
| | ATOM | 4181 | OH2 | H2O | 177 | 15.709 | 70.351 | -5.398 | 1.00 | 60.42 | W |
| | ATOM | 4182 | H1 | H2O | 177 | 15.048 | 70.541 | -4.731 | 1.00 | 0.00 | W |
| | ATOM | 4183 | H2 | H2O | 177 | 15.488 | 69.475 | -5.712 | 1.00 | 0.00 | W |
| | ATOM | 4184 | OH2 | H2O | 178 | 33.370 | 76.092 | 46.298 | 1.00 | 73.91 | W |
| 20 | ATOM | 4185 | H1 | H2O | 178 | 32.527 | 75.849 | 46.680 | 1.00 | 0.00 | W |
| | ATOM | 4186 | H2 | H2O | 178 | 33.647 | 76.862 | 46.791 | 1.00 | 0.00 | W |
| | ATOM | 4187 | OH2 | H2O | 179 | 32.160 | 88.256 | -3.330 | 1.00 | 31.03 | W |
| | ATOM | 4188 | H1 | H2O | 179 | 31.330 | 88.041 | -3.759 | 1.00 | 0.00 | W |
| | ATOM | 4189 | H2 | H2O | 179 | 32.571 | 88.893 | -3.916 | 1.00 | 0.00 | W |
| 25 | ATOM | 4190 | OH2 | H2O | 180 | 43.785 | 91.145 | 1.609 | 1.00 | 42.82 | W |
| | ATOM | 4191 | H1 | H2O | 180 | 44.441 | 91.779 | 1.325 | 1.00 | 0.00 | W |
| | ATOM | 4192 | H2 | H2O | 180 | 44.208 | 90.654 | 2.311 | 1.00 | 0.00 | W |
| | ATOM | 4193 | OH2 | H2O | 181 | 23.220 | 65.998 | 2.718 | 1.00 | 25.59 | W |
| | ATOM | 4194 | H1 | H2O | 181 | 22.845 | 66.784 | 2.330 | 1.00 | 0.00 | W |
| 30 | ATOM | 4195 | H2 | H2O | 181 | 22.846 | 65.275 | 2.212 | 1.00 | 0.00 | W |
| | ATOM | 4196 | OH2 | H2O | 182 | 7.003 | 43.420 | 24.621 | 1.00 | 50.96 | W |
| | ATOM | 4197 | H1 | H2O | 182 | 7.061 | 43.954 | 25.414 | 1.00 | 0.00 | W |
| | ATOM | 4198 | H2 | H2O | 182 | 7.912 | 43.254 | 24.376 | 1.00 | 0.00 | W |
| | ATOM | 4199 | OH2 | H2O | 183 | 27.129 | 44.901 | 42.342 | 1.00 | 61.07 | W |
| 35 | ATOM | 4200 | H1 | H2O | 183 | 26.349 | 45.392 | 42.607 | 1.00 | 0.00 | W |
| | ATOM | 4201 | H2 | H2O | 183 | 27.383 | 44.415 | 43.126 | 1.00 | 0.00 | W |
| | ATOM | 4202 | OH2 | H2O | 184 | 20.120 | 62.615 | 6.341 | 1.00 | 52.42 | W |
| | ATOM | 4203 | H1 | H2O | 184 | 19.717 | 63.462 | 6.535 | 1.00 | 0.00 | W |
| | ATOM | 4204 | H2 | H2O | 184 | 20.224 | 62.197 | 7.197 | 1.00 | 0.00 | W |
| 40 | ATOM | 4205 | OH2 | H2O | 186 | 10.038 | 94.189 | -8.999 | 1.00 | 40.69 | W |
| | ATOM | 4206 | H1 | H2O | 186 | 10.000 | 93.361 | -9.481 | 1.00 | 0.00 | W |
| | ATOM | 4207 | H2 | H2O | 186 | 9.190 | 94.600 | -9.161 | 1.00 | 0.00 | W |
| | ATOM | 4208 | OH2 | H2O | 187 | 39.048 | 78.109 | 48.627 | 1.00 | 43.94 | W |
| | ATOM | 4209 | H1 | H2O | 187 | 39.049 | 79.067 | 48.627 | 1.00 | 0.00 | W |
| 45 | ATOM | 4210 | H2 | H2O | 187 | 39.049 | 77.870 | 47.700 | 1.00 | 0.00 | W |
| | ATOM | 4211 | OH2 | H2O | 188 | 29.997 | 88.546 | 37.175 | 1.00 | 66.02 | W |
| | ATOM | 4212 | H1 | H2O | 188 | 29.998 | 89.503 | 37.176 | 1.00 | 0.00 | W |
| | ATOM | 4213 | H2 | H2O | 188 | 29.998 | 88.306 | 36.249 | 1.00 | 0.00 | W |
| | ATOM | 4214 | OH2 | H2O | 189 | 33.213 | 66.563 | 16.332 | 1.00 | 62.88 | W |
| 50 | ATOM | 4215 | H1 | H2O | 189 | 33.911 | 66.201 | 15.788 | 1.00 | 0.00 | W |
| | ATOM | 4216 | H2 | H2O | 189 | 33.092 | 67.455 | 16.008 | 1.00 | 0.00 | W |
| | ATOM | 4217 | OH2 | H2O | 190 | 29.894 | 60.575 | 22.671 | 1.00 | 41.27 | W |
| | ATOM | 4218 | H1 | H2O | 190 | 29.363 | 61.361 | 22.549 | 1.00 | 0.00 | W |
| | ATOM | 4219 | H2 | H2O | 190 | 30.767 | 60.909 | 22.889 | 1.00 | 0.00 | W |
| 55 | ATOM | 4220 | OH2 | H2O | 191 | 17.276 | 53.069 | 43.250 | 1.00 | 10.66 | W |
| | ATOM | 4221 | H1 | H2O | 191 | 17.592 | 53.312 | 44.119 | 1.00 | 0.00 | W |
| | ATOM | 4222 | H2 | H2O | 191 | 18.045 | 52.689 | 42.817 | 1.00 | 0.00 | W |
| | ATOM | 4223 | OH2 | H2O | 192 | 35.647 | 59.655 | 27.750 | 1.00 | 26.14 | W |
| | ATOM | 4224 | H1 | H2O | 192 | 36.404 | 59.816 | 28.311 | 1.00 | 0.00 | W |
| 60 | ATOM | 4225 | H2 | H2O | 192 | 35.899 | 60.010 | 26.897 | 1.00 | 0.00 | W |
| | ATOM | 4226 | OH2 | H2O | 193 | 38.775 | 60.787 | 30.053 | 1.00 | 36.89 | W |
| | ATOM | 4227 | H1 | H2O | 193 | 38.108 | 61.130 | 29.455 | 1.00 | 0.00 | W |
| | ATOM | 4228 | H2 | H2O | 193 | 39.557 | 61.302 | 29.857 | 1.00 | 0.00 | W |
| | ATOM | 4229 | OH2 | H2O | 194 | 18.790 | 80.718 | 52.778 | 1.00 | 28.10 | W |
| 65 | ATOM | 4230 | H1 | H2O | 194 | 18.791 | 81.672 | 52.780 | 1.00 | 0.00 | W |
| | ATOM | 4231 | H2 | H2O | 194 | 18.791 | 80.475 | 51.853 | 1.00 | 0.00 | W |
| | ATOM | 4232 | OH2 | H2O | 195 | 22.571 | 68.265 | 53.229 | 1.00 | 34.42 | W |
| | ATOM | 4233 | H1 | H2O | 195 | 23.152 | 67.936 | 53.916 | 1.00 | 0.00 | W |
| | ATOM | 4234 | H2 | H2O | 195 | 22.266 | 69.110 | 53.558 | 1.00 | 0.00 | W |
| 70 | ATOM | 4235 | OH2 | H2O | 196 | 7.904 | 98.993 | -8.160 | 1.00 | 39.75 | W |
| | ATOM | 4236 | H1 | H2O | 196 | 7.904 | 99.952 | -8.160 | 1.00 | 0.00 | W |
| | ATOM | 4237 | H2 | H2O | 196 | 7.904 | 98.755 | -9.087 | 1.00 | 0.00 | W |
| | ATOM | 4238 | OH2 | H2O | 197 | 15.117 | 76.593 | 49.958 | 1.00 | 44.24 | W |
| | ATOM | 4239 | H1 | H2O | 197 | 14.700 | 76.989 | 50.724 | 1.00 | 0.00 | W |
| | ATOM | 4240 | H2 | H2O | 197 | 15.264 | 77.325 | 49.360 | 1.00 | 0.00 | W |
| | ATOM | 4241 | OH2 | H2O | 198 | 18.738 | 61.062 | 5.012 | 1.00 | 57.29 | W |
| | ATOM | 4242 | H1 | H2O | 198 | 18.739 | 62.019 | 5.011 | 1.00 | 0.00 | W |

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| | | | | | | | | | | | |
|----|------|------|-----|-----|-----|--------|---------|--------|------|-------|---|
| | ATOM | 4243 | H2 | H2O | 198 | 18.739 | 60.822 | 4.084 | 1.00 | 0.00 | W |
| | ATOM | 4244 | OH2 | H2O | 199 | 38.023 | 88.017 | 8.921 | 1.00 | 34.68 | W |
| | ATOM | 4245 | H1 | H2O | 199 | 37.201 | 88.224 | 9.366 | 1.00 | 0.00 | W |
| | ATOM | 4246 | H2 | H2O | 199 | 37.785 | 87.348 | 8.278 | 1.00 | 0.00 | W |
| 5 | ATOM | 4247 | OH2 | H2O | 200 | 25.176 | 78.050 | 39.750 | 1.00 | 36.28 | W |
| | ATOM | 4248 | H1 | H2O | 200 | 25.349 | 78.069 | 38.807 | 1.00 | 0.00 | W |
| | ATOM | 4249 | H2 | H2O | 200 | 24.306 | 78.440 | 39.840 | 1.00 | 0.00 | W |
| | ATOM | 4250 | OH2 | H2O | 201 | 36.509 | 75.837 | 18.830 | 1.00 | 40.11 | W |
| 10 | ATOM | 4251 | H1 | H2O | 201 | 36.944 | 75.281 | 19.473 | 1.00 | 0.00 | W |
| | ATOM | 4252 | H2 | H2O | 201 | 36.226 | 76.605 | 19.326 | 1.00 | 0.00 | W |
| | ATOM | 4253 | OH2 | H2O | 202 | 15.114 | 86.425 | 44.318 | 1.00 | 26.14 | W |
| | ATOM | 4254 | H1 | H2O | 202 | 14.743 | 86.504 | 43.441 | 1.00 | 0.00 | W |
| | ATOM | 4255 | H2 | H2O | 202 | 15.979 | 86.832 | 44.251 | 1.00 | 0.00 | W |
| | ATOM | 4256 | OH2 | H2O | 203 | 34.096 | 66.512 | 23.788 | 1.00 | 48.56 | W |
| 15 | ATOM | 4257 | H1 | H2O | 203 | 34.012 | 66.195 | 24.690 | 1.00 | 0.00 | W |
| | ATOM | 4258 | H2 | H2O | 203 | 34.943 | 66.959 | 23.773 | 1.00 | 0.00 | W |
| | ATOM | 4259 | OH2 | H2O | 204 | 28.998 | 83.540 | 37.915 | 1.00 | 48.28 | W |
| | ATOM | 4260 | H1 | H2O | 204 | 29.160 | 83.028 | 37.122 | 1.00 | 0.00 | W |
| 20 | ATOM | 4261 | H2 | H2O | 204 | 29.874 | 83.729 | 38.257 | 1.00 | 0.00 | W |
| | ATOM | 4262 | OH2 | H2O | 205 | 36.771 | 86.241 | 17.583 | 1.00 | 28.64 | W |
| | ATOM | 4263 | H1 | H2O | 205 | 37.720 | 86.287 | 17.698 | 1.00 | 0.00 | W |
| | ATOM | 4264 | H2 | H2O | 205 | 36.608 | 86.681 | 16.750 | 1.00 | 0.00 | W |
| | ATOM | 4265 | OH2 | H2O | 206 | 34.304 | 83.977 | 22.394 | 1.00 | 37.11 | W |
| 25 | ATOM | 4266 | H1 | H2O | 206 | 33.908 | 83.964 | 23.266 | 1.00 | 0.00 | W |
| | ATOM | 4267 | H2 | H2O | 206 | 33.588 | 84.238 | 21.812 | 1.00 | 0.00 | W |
| | ATOM | 4268 | OH2 | H2O | 207 | 10.426 | 85.642 | 38.336 | 1.00 | 35.00 | W |
| | ATOM | 4269 | H1 | H2O | 207 | 10.276 | 85.151 | 39.144 | 1.00 | 0.00 | W |
| | ATOM | 4270 | H2 | H2O | 207 | 10.589 | 86.537 | 38.626 | 1.00 | 0.00 | W |
| 30 | ATOM | 4271 | OH2 | H2O | 208 | 33.164 | 40.493 | 36.564 | 1.00 | 43.55 | W |
| | ATOM | 4272 | H1 | H2O | 208 | 33.931 | 39.992 | 36.285 | 1.00 | 0.00 | W |
| | ATOM | 4273 | H2 | H2O | 208 | 32.453 | 40.170 | 36.012 | 1.00 | 0.00 | W |
| | ATOM | 4274 | OH2 | H2O | 209 | 9.667 | 59.806 | 49.799 | 1.00 | 27.66 | W |
| | ATOM | 4275 | H1 | H2O | 209 | 9.078 | 59.514 | 49.107 | 1.00 | 0.00 | W |
| 35 | ATOM | 4276 | H2 | H2O | 209 | 10.523 | 59.452 | 49.554 | 1.00 | 0.00 | W |
| | ATOM | 4277 | OH2 | H2O | 210 | 40.620 | 91.683 | 9.844 | 1.00 | 44.74 | W |
| | ATOM | 4278 | H1 | H2O | 210 | 39.757 | 91.357 | 10.104 | 1.00 | 0.00 | W |
| | ATOM | 4279 | H2 | H2O | 210 | 40.905 | 91.080 | 9.157 | 1.00 | 0.00 | W |
| | ATOM | 4280 | OH2 | H2O | 211 | 31.114 | 53.143 | 38.106 | 1.00 | 19.43 | W |
| 40 | ATOM | 4281 | H1 | H2O | 211 | 30.669 | 52.292 | 38.079 | 1.00 | 0.00 | W |
| | ATOM | 4282 | H2 | H2O | 211 | 31.806 | 53.073 | 37.457 | 1.00 | 0.00 | W |
| | ATOM | 4283 | OH2 | H2O | 212 | 37.410 | 58.585 | 24.168 | 1.00 | 51.69 | W |
| | ATOM | 4284 | H1 | H2O | 212 | 36.615 | 59.088 | 23.990 | 1.00 | 0.00 | W |
| | ATOM | 4285 | H2 | H2O | 212 | 37.097 | 57.750 | 24.508 | 1.00 | 0.00 | W |
| 45 | ATOM | 4286 | OH2 | H2O | 213 | 37.530 | 82.337 | 17.584 | 1.00 | 25.73 | W |
| | ATOM | 4287 | H1 | H2O | 213 | 36.642 | 81.987 | 17.649 | 1.00 | 0.00 | W |
| | ATOM | 4288 | H2 | H2O | 213 | 38.090 | 81.564 | 17.520 | 1.00 | 0.00 | W |
| | ATOM | 4289 | OH2 | H2O | 214 | 20.562 | 62.057 | 49.243 | 1.00 | 36.13 | W |
| | ATOM | 4290 | H1 | H2O | 214 | 20.191 | 62.888 | 48.941 | 1.00 | 0.00 | W |
| 50 | ATOM | 4291 | H2 | H2O | 214 | 20.159 | 61.398 | 48.677 | 1.00 | 0.00 | W |
| | ATOM | 4292 | OH2 | H2O | 215 | 38.487 | 67.744 | 46.984 | 1.00 | 28.08 | W |
| | ATOM | 4293 | H1 | H2O | 215 | 38.487 | 68.698 | 46.981 | 1.00 | 0.00 | W |
| | ATOM | 4294 | H2 | H2O | 215 | 38.487 | 67.501 | 46.054 | 1.00 | 0.00 | W |
| | ATOM | 4295 | OH2 | H2O | 216 | 4.672 | 50.241 | 43.410 | 1.00 | 37.85 | W |
| 55 | ATOM | 4296 | H1 | H2O | 216 | 3.799 | 49.905 | 43.616 | 1.00 | 0.00 | W |
| | ATOM | 4297 | H2 | H2O | 216 | 5.068 | 50.420 | 44.262 | 1.00 | 0.00 | W |
| | ATOM | 4298 | OH2 | H2O | 217 | 32.087 | 71.911 | 7.975 | 1.00 | 35.72 | W |
| | ATOM | 4299 | H1 | H2O | 217 | 32.492 | 72.674 | 7.563 | 1.00 | 0.00 | W |
| | ATOM | 4300 | H2 | H2O | 217 | 31.862 | 72.205 | 8.857 | 1.00 | 0.00 | W |
| 60 | ATOM | 4301 | OH2 | H2O | 218 | 37.077 | 71.241 | 31.371 | 1.00 | 28.59 | W |
| | ATOM | 4302 | H1 | H2O | 218 | 36.181 | 71.414 | 31.087 | 1.00 | 0.00 | W |
| | ATOM | 4303 | H2 | H2O | 218 | 37.354 | 70.488 | 30.847 | 1.00 | 0.00 | W |
| | ATOM | 4304 | OH2 | H2O | 219 | 12.531 | 78.336 | 47.863 | 1.00 | 38.31 | W |
| | ATOM | 4305 | H1 | H2O | 219 | 11.632 | 78.370 | 47.538 | 1.00 | 0.00 | W |
| | ATOM | 4306 | H2 | H2O | 219 | 12.440 | 78.304 | 48.816 | 1.00 | 0.00 | W |
| 65 | ATOM | 4307 | OH2 | H2O | 236 | 5.922 | 55.713 | 49.951 | 1.00 | 34.41 | W |
| | ATOM | 4308 | H1 | H2O | 236 | 6.664 | 55.901 | 49.382 | 1.00 | 0.00 | W |
| | ATOM | 4309 | H2 | H2O | 236 | 6.297 | 55.224 | 50.679 | 1.00 | 0.00 | W |
| | ATOM | 4310 | OH2 | H2O | 237 | 32.810 | 50.612 | 40.203 | 1.00 | 42.20 | W |
| 70 | ATOM | 4311 | H1 | H2O | 237 | 32.021 | 51.115 | 40.399 | 1.00 | 0.00 | W |
| | ATOM | 4312 | H2 | H2O | 237 | 32.497 | 49.728 | 40.026 | 1.00 | 0.00 | W |
| | ATOM | 4313 | OH2 | H2O | 238 | 16.579 | 101.122 | -4.447 | 1.00 | 38.51 | W |
| | ATOM | 4314 | H1 | H2O | 238 | 15.993 | 101.299 | -5.184 | 1.00 | 0.00 | W |
| | ATOM | 4315 | H2 | H2O | 238 | 16.974 | 100.276 | -4.652 | 1.00 | 0.00 | W |

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|---|------|------|-----|-----|-----|--------|--------|---------|------|-------|---|
| 5 | ATOM | 4316 | OH2 | H2O | 239 | 17.874 | 69.091 | 56.692 | 1.00 | 38.94 | W |
| | ATOM | 4317 | H1 | H2O | 239 | 17.874 | 70.049 | 56.691 | 1.00 | 0.00 | W |
| | ATOM | 4318 | H2 | H2O | 239 | 17.874 | 68.852 | 55.764 | 1.00 | 0.00 | W |
| | ATOM | 4319 | OH2 | H2O | 240 | 12.249 | 77.436 | -11.341 | 1.00 | 40.18 | W |
| | ATOM | 4320 | H1 | H2O | 240 | 12.960 | 78.076 | -11.282 | 1.00 | 0.00 | W |
| | ATOM | 4321 | H2 | H2O | 240 | 12.370 | 77.023 | -12.196 | 1.00 | 0.00 | W |
| | ATOM | 4322 | OH2 | H2O | 241 | 29.087 | 65.635 | 23.981 | 1.00 | 33.57 | W |
| | ATOM | 4323 | H1 | H2O | 241 | 28.790 | 65.725 | 24.885 | 1.00 | 0.00 | W |
| | ATOM | 4324 | H2 | H2O | 241 | 29.863 | 66.198 | 23.928 | 1.00 | 0.00 | W |